

chain nodes :

9

ring nodes :

2 3 4 5 6 7 8

ring/chain nodes :

10 12 13 15

chain bonds :

2-15 5-12 6-13 8-9

ring/chain bonds :

3-10

ring bonds :

2-3 2-8 3-4 4-5 5-6 6-7 7-8

exact/norm bonds :

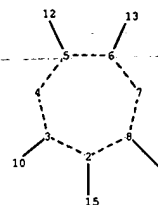
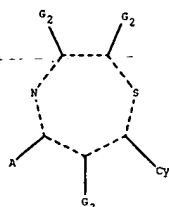
2-3 2-8 2-15 3-4 3-10 4-5 5-6 5-12 6-7 6-13 7-8 8-9

G1:O,S,N

G2:A,H

Match level :

2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:CLASS  
12:CLASS 13:CLASS 15:CLASS



chain nodes :

9

ring nodes :

2 3 4 5 6 7 8

ring/chain nodes :

10 12 13 15

chain bonds :

2-15 8-9

ring/chain bonds :

3-10 5-12 6-13

ring bonds :

2-3 2-8 3-4 4-5 5-6 6-7 7-8

exact/norm bonds :

2-3 2-8 2-15 3-4 3-10 4-5 5-6 5-12 6-7 6-13 7-8 8-9

G1:O,S,N

G2:A,H

Match level :

2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:CLASS  
12:CLASS 13:CLASS 15:CLASS

09/836,548

=> d his

(FILE 'HOME' ENTERED AT 12:57:35 ON 30 OCT 2002)

FILE 'REGISTRY' ENTERED AT 12:57:43 ON 30 OCT 2002

FILE 'STNGUIDE' ENTERED AT 13:01:01 ON 30 OCT 2002

FILE 'REGISTRY' ENTERED AT 13:04:21 ON 30 OCT 2002

L1 STRUCTURE UPLOADED  
L2 QUE L1  
L3 21 S L2  
L4 1885 S L2 SSS FUL  
L5 STRUCTURE UPLOADED  
L6 QUE L5  
L7 11 S L6 SUB=L4 SAM  
L8 185 S L6 SUB=L4 FUL *thiazepines*  
L9 1700 S L4 NOT L8  
L10 9574 S C6-C5NS/EA  
L11 1373 S L9 AND L10 *benzothiazepines*  
L12 327 S L9 NOT L11 *polycyclics*

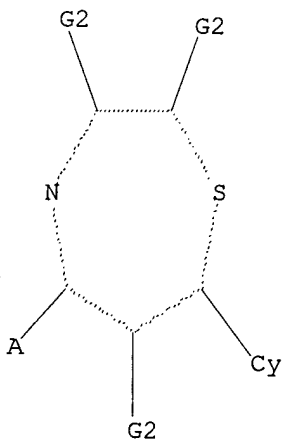
FILE 'CAPLUS' ENTERED AT 13:11:37 ON 30 OCT 2002

L13 21 S L8  
L14 426 S L11  
L15 80 S L12  
SAVE L14 A09836548/A  
SAVE L15 B09836548/A

=> d 12

L2 HAS NO ANSWERS

L1 STR



G1 O, S, N

G2 A, H

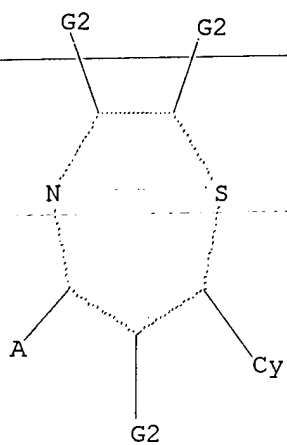
Structure attributes must be viewed using STN Express query preparation.

L2 QUE ABB=ON PLU=ON L1

=> d 15

09/836,548

L5 HAS NO ANSWERS  
L5 STR



G1 O, S, N

G2 A, H

Structure attributes must be viewed using STN Express query preparation.

=> d ibib abs hitstr 113 1-21

~~118~~ ANSWER 1 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:293652 CAPLUS

DOCUMENT NUMBER: 136:325531

TITLE: Preparation of (poly)azanaphthalenyl carboxamides as HIV integrase inhibitors

INVENTOR(S): Anthony, Neville J.; Gomez, Robert P.; Young, Steven D.; Egbertson, Melissa; Wai, John S.; Zhuang, Linghang; Embrey, Mark; Tran, Lekhanh; Melamed, Jeffrey Y.; Langford, H. Marie; Guare, James P.; Fisher, Thorsten E.; Jolly, Samson M.; Kuo, Michelle S.; Perlow, Debra S.; Bennett, Jennifer J.; Funk, Timothy W.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 434 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

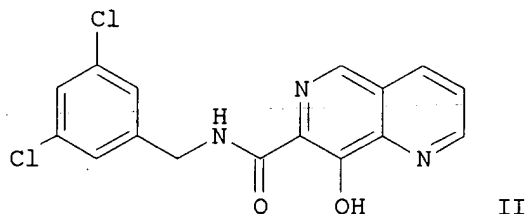
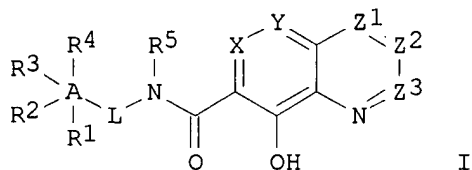
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

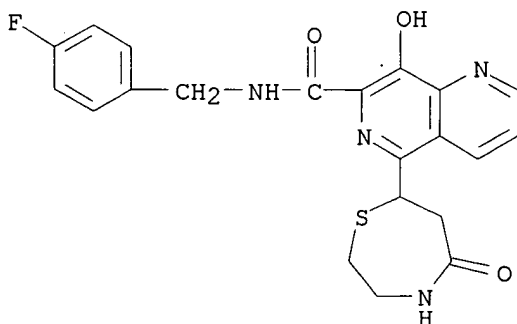
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002030930	A2	20020418	WO 2001-US31456	20011009
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002011527	A5	20020422	AU 2002-11527	20011009
PRIORITY APPLN. INFO.:			US 2000-239707P	P 20001012
			US 2001-281656P	P 20010405
			WO 2001-US31456	W 20011009

OTHER SOURCE(S): MARPAT 136:325531

GI



- AB Title compds., including certain quinoline carboxamide and naphthyridine carboxamide derivs., I [wherein A = (un)substituted Ph or Ph fused to a carbocycle; L = a single bond, or (un)substituted alkyl, alkenyl, alkylcycloalkylalkyl, or alkyl-M-alkyl; M = NRa, OCO, or CO<sub>2</sub>; X = N or CQ1; Y = N or CQ2, provided that X and Y are not both N; Z1 = N or CQ3; Z2 = N or CQ4; Z3 = N or CH; Q1-Q4 = independently H, halo, CN, NR1CR10, or (un)substituted alkyl, alkoxy, alkenyl, alkynyl, carbamoyl, carboximidamido, amino, etc.; or C2Q2Q3 = (un)substituted 5- or 6-membered carbocycle or heterocycle; R1 and R2 = independently H, OH, halo, NO<sub>2</sub>, CN, or (un)substituted alkyl, alkenyl, alkoxy, amino, sulfonylamino, etc.; R3 and R4 = independently H, halo, CN, NO<sub>2</sub>, OH, alkenyl, or (un)substituted alkyl, amino, sulfonylamino, etc.; R5 = H, CN, CN, or (un)substituted alkyl or aryl; Ra = independently H or (halo)alkyl; or pharmaceutically acceptable salts thereof] were prepd. I are inhibitors of HIV integrase and inhibitors of HIV replication, and are useful in the prevention or treatment of infection by HIV and the treatment of AIDS, as compds. or pharmaceutically acceptable salts, or as ingredients in pharmaceutical compns., optionally in combination with other antivirals, immunomodulators, antibiotics, or vaccines. For example, Mitsunobu reaction of iso-Pr 3-(hydroxymethyl)pyridine-2-carboxylate with Me N-[(4-methylphenyl)sulfonyl]glycinate, followed by cyclization in the presence on NaOMe, afforded Me 8-hydroxy-1,6-naphthyridine-7-carboxylate. Coupling with 3,5-dichlorobenzylamine in toluene gave II. Representative compds. were assayed for the inhibition of acute HIV infection of T-lymphoid cells and demonstrated IC<sub>95</sub> values of < 20 .mu.M.
- IT **410544-78-4P**, N-(4-Fluorobenzyl)-8-hydroxy-5-(5-oxo-1,4-thiazepan-7-yl)[1,6]naphthyridine-7-carboxamide  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (HIV integrase inhibitor; prepn. of (poly)azanaphthalenyl carboxamides as HIV integrase inhibitors for treatment of AIDS)
- RN 410544-78-4 CAPLUS
- CN 1,6-Naphthyridine-7-carboxamide, N-[(4-fluorophenyl)methyl]-5-(hexahydro-5-oxo-1,4-thiazepin-7-yl)-8-hydroxy- (9CI) (CA INDEX NAME)



- IT **410544-79-5P**, N-(4-Fluorobenzyl)-8-hydroxy-5-(1-oxido-5-oxo-1,4-thiazepan-7-yl)-[1,6]naphthyridine-7-carboxamide **410544-80-8P**, N-(4-Fluorobenzyl)-8-hydroxy-5-(1,1-dioxido-5-oxo-1,4-thiazepan-7-yl)[1,6]naphthyridine-7-carboxamide  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

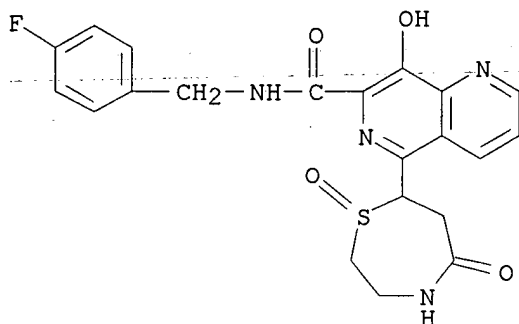
09/836,548

(Uses)

(HIV integrase inhibitor; prepn. of (poly)azanaphthalenyl carboxamides  
as HIV integrase inhibitors for treatment of AIDS)

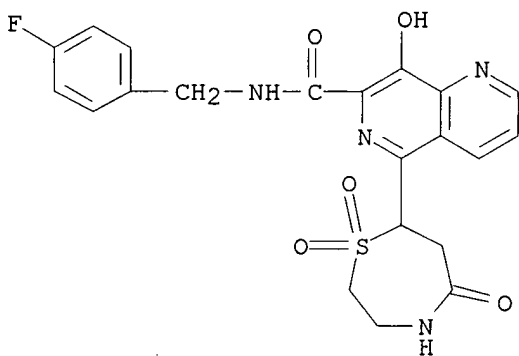
RN 410544-79-5 CAPLUS

CN 1,6-Naphthyridine-7-carboxamide, N-[(4-fluorophenyl)methyl]-5-(hexahydro-1-  
oxido-5-oxo-1,4-thiazepin-7-yl)-8-hydroxy- (9CI) (CA INDEX NAME)



RN 410544-80-8 CAPLUS

CN 1,6-Naphthyridine-7-carboxamide, N-[(4-fluorophenyl)methyl]-5-(hexahydro-  
1,1-dioxido-5-oxo-1,4-thiazepin-7-yl)-8-hydroxy- (9CI) (CA INDEX NAME)



133 ANSWER 2 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:869523 CAPLUS

DOCUMENT NUMBER: 136:161045

TITLE: Inhibition of P-selectin specific cell adhesion by a low molecular weight, non-carbohydrate compound, KF38789

AUTHOR(S): Ohta, S.; Inujima, Y.; Abe, M.; Uosaki, Y.; Sato, S.; Miki, I.

CORPORATE SOURCE: Department of Immunology, Drug Research Laboratories, Pharmaceutical Research Institute, Kyowa Hakko Kogyo Co., Ltd., Shizuoka, 411-8731, Japan

SOURCE: Inflammation Research (2001), 50(11), 544-551  
CODEN: INREFB; ISSN: 1023-3830

PUBLISHER: Birkhaeuser Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Objective and design: P-selectin is a cell adhesion mol. of the selectin family. This study evaluated the effects of novel, low mol. wt. P-selectin inhibitors in a cell adhesion assay and a murine model of peritonitis. Materials: U937 or HL60 was used for cell adhesion assay. Human polymorphonuclear cells were studied for the prodn. of superoxide. BALB/c mice were used for the in vivo study. Treatment: The thioglycollate (TG)-induced accumulation of leukocytes in mice was measured 6 h after the treatment. KF38789 or antibody (1 mg/kg) was injected i.v. prior to TG injection and at 3 h following initial injection. Results: Low mol. wt., non-carbohydrate inhibitors against P-selectin-mediated cell adhesion were tested. One of the most potent inhibitors, KF38789, inhibited the binding of U937 cells to immobilized P-selectin IgG chimeric protein (P-selectin-Ig) with an IC50 value of 1.97 .mu.M. Cell adhesion to both E-selectin-Ig and L-selectin-Ig were not affected even by 100 .mu.M of KF38789. Moreover, KF38789 inhibited P-selectin-induced superoxide prodn. from human polymorphonuclear cells. I.v. injected KF38789 significantly inhibited the TG-induced accumulation of leukocytes in the mouse peritoneal cavity (p<0.01). Conclusion: A novel low mol. wt. compd., KF38789, specifically inhibited P-selectin-dependent cell adhesion and the leukocyte recruitment in mouse peritonitis.

IT 257292-28-7 257292-29-8, KF 38789 257292-30-1  
257292-31-2 257292-33-4 257292-34-5  
257292-36-7 257292-38-9 257292-41-4  
257292-44-7

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

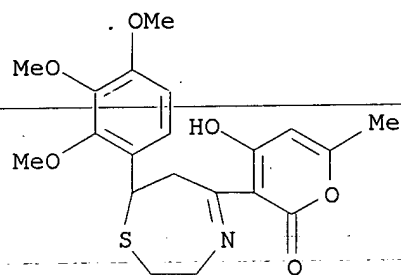
(inhibition of P-selectin specific cell adhesion by a low mol. wt., non-carbohydrate compd., KF38789)

RN 257292-28-7 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)

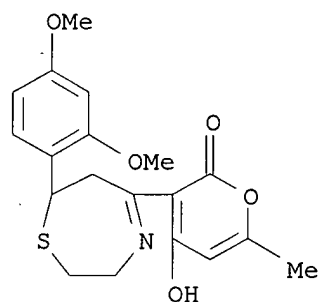


09/836,548



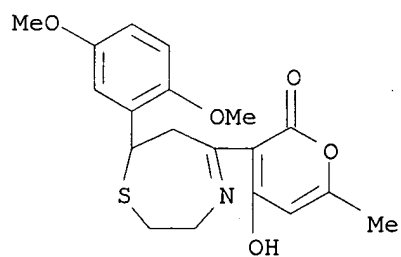
RN 257292-29-8 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



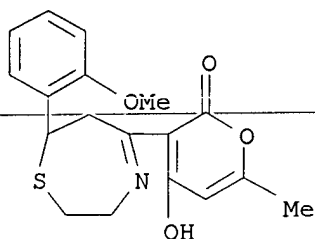
RN 257292-30-1 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,5-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

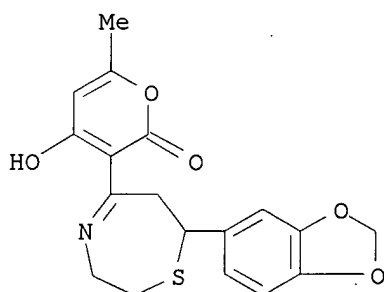


RN 257292-31-2 CAPLUS

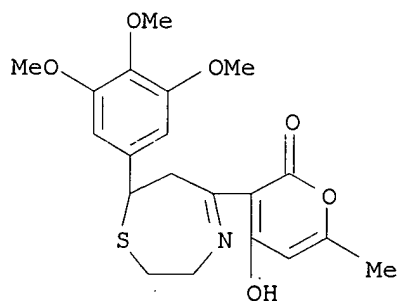
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



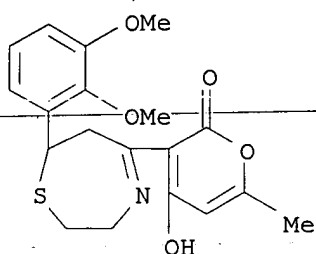
RN 257292-33-4 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-(1,3-benzodioxol-5-yl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 257292-34-5 CAPLUS  
 CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3,4,5-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)

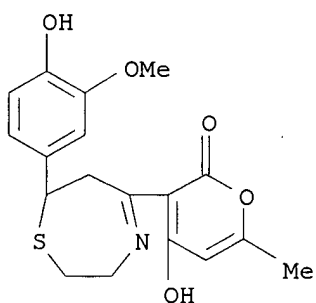


RN 257292-36-7 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-(2,3-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



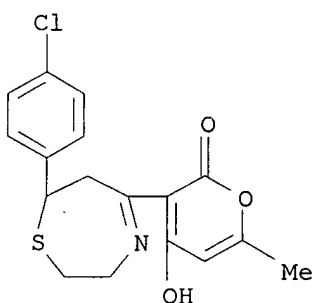
RN 257292-38-9 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-hydroxy-3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 257292-41-4 CAPLUS

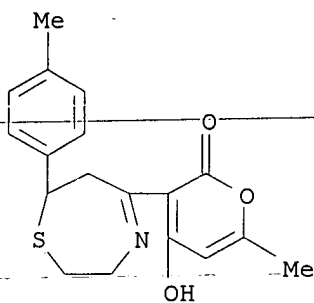
CN 2H-Pyran-2-one, 3-[7-(4-chlorophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 257292-44-7 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-methylphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)

09/836,548



REFERENCE COUNT:

38

THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:780869 CAPLUS

DOCUMENT NUMBER: 135:331449

TITLE: Preparation of substituted 1,4-thiazepines and analogs  
as activators of caspases and inducers of apoptosis  
for treatment of cancer and other proliferative  
diseases

INVENTOR(S): Cai, Sui Xiong; Drewe, John A.; Shelton, Emma Jane;  
Litvak, Joane; Sperandio, David; Spencer, Jeffrey R.

PATENT ASSIGNEE(S): Cytovia, Inc., USA

SOURCE: PCT Int. Appl., 162 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001079187	A2	20011025	WO 2001-US12581	20010418
WO 2001079187	A3	20020221		

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CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,  
HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,  
LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,  
RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ,  
VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

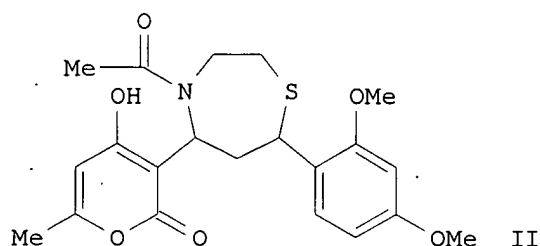
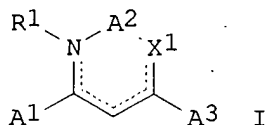
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DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2002010169	A1	20020124	US 2001-836548	20010418
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PRIORITY APPLN. INFO.: US 2000-197599P P 20000418

OTHER SOURCE(S): MARPAT 135:331449

GI



AB Title compds. I [wherein R1 = null, H, alkyl, or COR6; X1 = NR2, S, SO, SO2, or O; R6 = null, H, or (halo)alkyl; A1 = (un)substituted monocyclic or fused polycyclic (hetero)aryl or (hetero)cycloalkyl ring; or A1 and R1 together form an (un)substituted fused polycyclic heteroaryl or heterocycloalkyl ring; the ring contg. A2 = (un)substituted monocyclic or fused bicyclic heteroarylene or heterocycloalkylene ring; A3 = (un)substituted monocyclic or fused polycyclic (hetero)aryl or (hetero)cycloalkyl ring; and N-oxides, prodrugs, protected derivs.,

stereoisomers, and pharmaceutically acceptable salts thereof] were prepd. as caspase activators and apoptosis inducers. For example, coupling of 3-acetyl-4-hydroxy-6-methylpyran-2-one with 2,4-dimethoxybenzaldehyde, followed by cyclization with 2-aminoethanethiol (61%) and acetylation, gave the [1,4]thiazepine II. Five invention compds. were tested and demonstrated caspase potency in human breast cancer cell lines T-47D and ZR-75-1 with EC50 values ranging from 345 nM to 6930 nM and 163 nM to 4207 nM, resp. Thus, I and their compns. with known cancer chemotherapeutic agents are useful for the treatment of drug resistant cancer in animals.

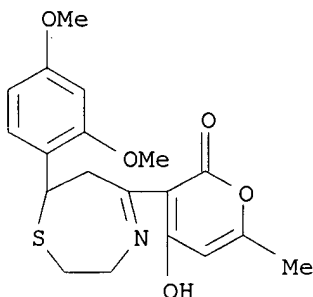
IT **257292-29-8P**, 3-[7-(2,4-Dimethoxyphenyl)-2,3,6,7-tetrahydro-  
[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of substituted 1,4-thiazepines and analogs as activators of caspases and inducers of apoptosis for treatment of cancer and other proliferative diseases)

RN 257292-29-8 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



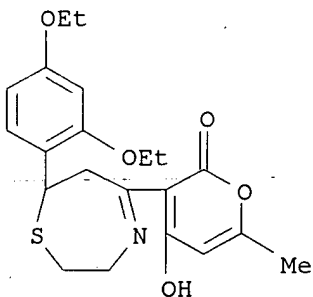
IT **369388-77-2P**, 4-Hydroxy-3-[7-(2,4-diethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-6-methylpyran-2-one

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of substituted 1,4-thiazepines and analogs as activators of caspases and inducers of apoptosis for treatment of cancer and other proliferative diseases)

RN 369388-77-2 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,4-diethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



IT 331852-70-1P, 3-[7-(2,3-Dichlorophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]4-hydroxy-6-methylpyran-2-one 331857-68-2P, 4-Hydroxy-6-methyl-3-[7-(4-methylthiophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one 331857-79-5P, 3-[7-(4-Ethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 331857-86-4P, 3-[7-(2-Bromophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]4-hydroxy-6-methylpyran-2-one 369387-63-3P, 4-Hydroxy-6-methyl-3-[7-(3-phenyl-1H-pyrazol-4-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one 369387-65-5P, 3-[7-(5-Ethylthien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-66-6P, 3-[7-(1-Benzyl-1H-indol-3-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-68-8P, 4-Hydroxy-6-methyl-3-[7-(2-trifluoromethylthiophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one 369387-69-9P, 4-Hydroxy-6-methyl-3-[7-(3-trifluoromethylthiophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one 369387-71-3P, 4-Hydroxy-6-methyl-3-[7-(4-trifluoromethylthiophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one 369387-72-4P, 4-Hydroxy-6-methyl-3-[7-[3-(3-trifluoromethylphenoxy)phenyl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one 369387-74-6P, 3-[7-[3-(3,4-Dichlorophenoxy)phenyl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-76-8P, 3-[7-[3-(3,5-Dichlorophenoxy)phenyl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-77-9P, 4-Hydroxy-6-methyl-3-[7-[5-(3-trifluoromethylphenyl)furan-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one 369387-79-1P, 3-[7-[5-(2-Chlorophenyl)furan-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-80-4P, 3-[7-[5-(3-Chlorophenyl)furan-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-81-5P, 3-[7-[5-(4-Chlorophenyl)furan-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-82-6P, 4-Hydroxy-6-methyl-3-[7-[5-(2-chloro-5-trifluoromethylphenyl)furan-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one 369387-83-7P, 3-[7-(4-Bromothien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-84-8P, 3-[7-(5-Bromothien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-86-0P, 3-[7-(1-Benzylsulfonyl-1H-pyrrol-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-88-2P, 4-Hydroxy-6-methyl-3-[7-(3-methylthien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one 369387-89-3P, 4-Hydroxy-6-methyl-3-[7-(5-methylthien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one 369387-91-7P, 4-Hydroxy-6-methyl-3-[7-(1-methyl-1H-indol-3-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one 369387-93-9P, 3-[7-(3-Chloro-2-methyl-5-trifluoromethyl-1H-pyrazol-4-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-94-0P, 3-[7-[1-(2,4-Difluorobenzylsulfonyl)-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-96-2P, 3-(7-[2,2']Bithienyl-5-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-97-3P, 3-[7-[1-(3,5-Dichlorophenyl)-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369387-99-5P, 3-[7-[1-(4-Chlorophenyl)-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one 369388-00-1P 369388-03-4P, 4-Hydroxy-6-methyl-3-[7-(6-p-tolylthioimidazo[2,1-

b)thiazol-5-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one  
**369388-06-7P**, 3-[7-(4,5-Dibromothien-2-yl)-2,3,6,7-tetrahydro-  
 [1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-09-0P**,  
 4-Hydroxy-6-methyl-3-[7-(5-methylthiothien-2-yl)-2,3,6,7-tetrahydro-  
 [1,4]thiazepin-5-yl]pyran-2-one **369388-12-5P**,  
 3-[7-(5-Chloro-1-methyl-3-phenyl-1H-pyrazol-4-yl)-2,3,6,7-tetrahydro-  
 [1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-14-7P**,  
 3-[7-(4-Dimethylaminophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-  
 hydroxy-6-methylpyran-2-one **369388-15-8P**, 4-Hydroxy-6-methyl-3-  
 [7-(4-trifluoromethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-  
 2-one **369388-17-0P**, 4-Hydroxy-3-[7-(4-methylsulfonylphenyl)-  
 2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-6-methylpyran-2-one  
**369388-19-2P**, 3-[7-(2,4-Dimethoxyphenyl)-2,3,6,7-tetrahydro-  
 [1,4]thiazepin-5-yl]-4-methoxy-6-methylpyran-2-one **369388-21-6P**,  
 3-[7-(2,4-Dimethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-  
 hydroxy-6-methyl-5,6-dihydropyran-2-one **369388-23-8P**,  
 3-[7-(2,4-Diethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-  
 hydroxy-6-methyl-5,6-dihydropyran-2-one **369388-25-0P**,  
 3-[7-(4-Dimethylaminophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-  
 hydroxy-6-methyl-5,6-dihydropyran-2-one **369388-27-2P**,  
 3-[7-(2,3,4-Trimethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-  
 hydroxy-6-methyl-5,6-dihydropyran-2-one **369388-29-4P**  
**369388-31-8P 369388-33-0P 369388-35-2P**,  
 3-[7-(2,4-Dimethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-  
 hydroxy-1H-quinolin-2-one **369388-44-3P**, 3-[4-Acetyl-7-(2,4-  
 dimethoxyphenyl)[1,4]thiazepan-5-yl]-4-hydroxy-6-methylpyran-2-one  
**369388-46-5P**, 3-[7-(2,4-Dimethoxyphenyl)-4-(2,2,2-  
 trifluoroethanoyl)-[1,4]thiazepan-5-yl]-4-hydroxy-6-methylpyran-2-one  
**369388-48-7P**, 1-[7-(2,4-Dimethoxyphenyl)-5-(3-fluoro-4-  
 methoxyphenyl)-[1,4]thiazepan-4-yl]ethanone **369388-50-1P**,  
 3-[7-(2,4-Dimethoxyphenyl)-2,3-dihydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-  
 methylpyran-2-one **369388-52-3P**, 3-[7-(2,4-Diethoxyphenyl)-2,3-  
 dihydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one  
**369388-54-5P 369388-56-7P**, 3-[7-(2,4-Diethoxyphenyl)-2,3-  
 dihydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methyl-5,6-dihydropyran-2-one  
**369388-58-9P 369388-60-3P**, 3-[7-(2,4-Dimethoxyphenyl)-1-  
 oxo-2,3,6,7-tetrahydro-1H-1.lambd.4-[1,4]thiazepin-5-yl]-4-hydroxy-6-  
 methoxypyran-2-one **369388-62-5P 369388-67-0P**,  
 10-(2,4-Dimethoxyphenyl)-3-methyl-7,8-dihydro-10H-2,5-dioxa-9-thia-6a-  
 azacyclohepta[a]naphthalene-1,6-dione **369388-69-2P**,  
 4-Hydroxy-3-[7-(2-methoxy-4-methylthiophenyl)-2,3,6,7-tetrahydro-  
 [1,4]thiazepin-5-yl]-6-methylpyran-2-one **369388-71-6P**,  
 3-[7-(2-Chloro-5-trifluoromethylphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-  
 5-yl]-4-hydroxy-6-methylpyran-2-one **369388-73-8P**,  
 3-[7-(4-Dimethylamino-2-methoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-  
 yl]-4-hydroxy-6-methylpyran-2-one **369388-75-0P**,  
 4-Hydroxy-3-[7-(4-chloro-2-methoxyphenyl)-2,3,6,7-tetrahydro-  
 [1,4]thiazepin-5-yl]-6-methylpyran-2-one **369388-79-4P**,  
 7-(2,4-Dimethoxyphenyl)-5-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)-2,2-  
 dimethyl-2,3,6,7-tetrahydro-[1,4]thiazepine-3-carboxylic acid  
**369388-81-8P 369388-85-2P**, 3-[7-(3-Methoxyphenyl)-  
 2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-6-methylpyran-2-one  
**369388-89-6P**, 3-[7-(3,4-Dichlorophenyl)-2,3,6,7-tetrahydro-  
 [1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-91-0P**,  
 6-Methyl-3-[7-(2,3,4-trimethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-  
 yl]pyran-2-one **369389-71-9P**, 3-[7-(2,4-Dimethoxyphenyl)-1-oxo-  
 2,3,6,7-tetrahydro-1H-1.lambd.4-[1,4]thiazepin-5-yl]-4-hydroxy-6-  
 methylpyran-2-one **369389-72-0P**, 4-Hydroxy-6-methyl-3-[7-(3-



methoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one

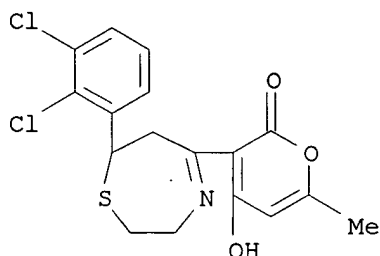
**369605-23-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted 1,4-thiazepines and analogs as activators of caspases and inducers of apoptosis for treatment of cancer and other proliferative diseases)

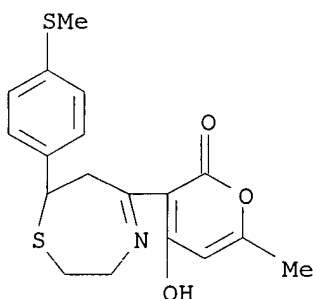
RN 331852-70-1 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,3-dichlorophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



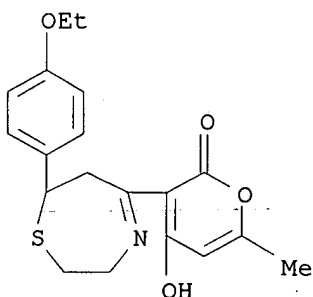
RN 331857-68-2 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-(methylthio)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 331857-79-5 CAPLUS

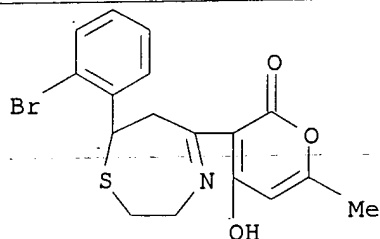
CN 2H-Pyran-2-one, 3-[7-(4-ethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



09/836,548

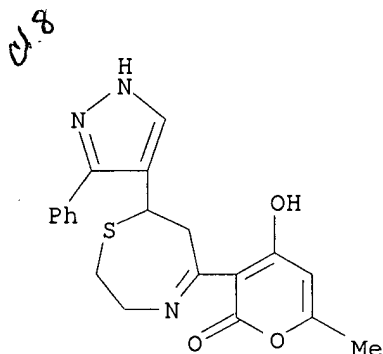
RN 331857-86-4 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2-bromophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



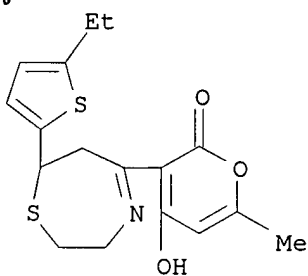
RN 369387-63-3 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3-phenyl-1H-pyrazol-4-yl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



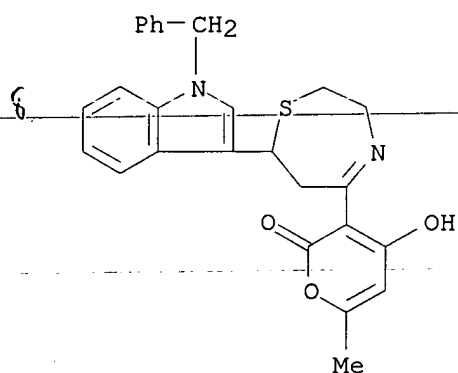
RN 369387-65-5 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(5-ethyl-2-thienyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

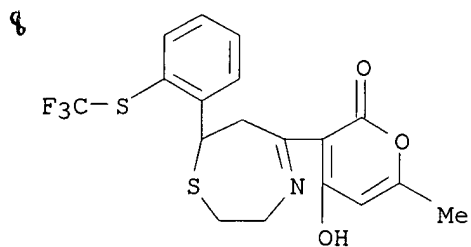


RN 369387-66-6 CAPLUS

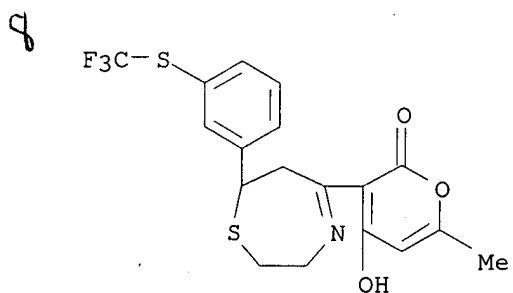
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[1-(phenylmethyl)-1H-indol-3-yl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



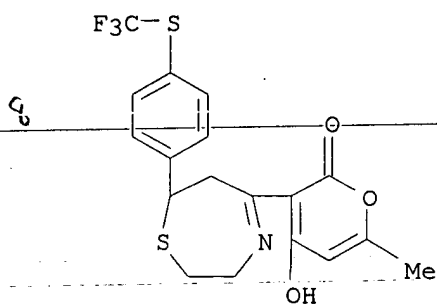
RN 369387-68-8 CAPLUS  
 CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[2-  
 [(trifluoromethyl)thio]phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 369387-69-9 CAPLUS  
 CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[3-  
 [(trifluoromethyl)thio]phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)

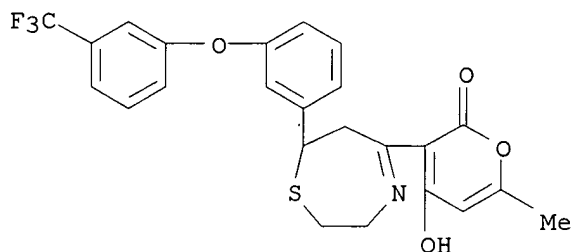


RN 369387-71-3 CAPLUS  
 CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-  
 [(trifluoromethyl)thio]phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



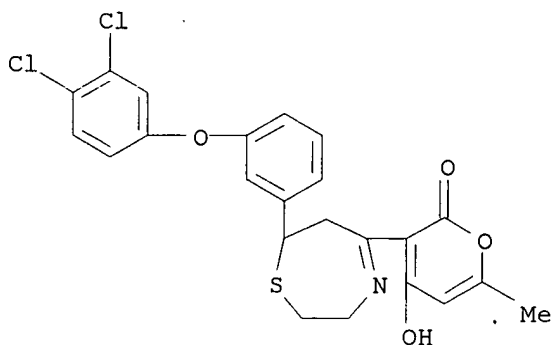
RN 369387-72-4 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[3-[3-(trifluoromethyl)phenoxy]phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



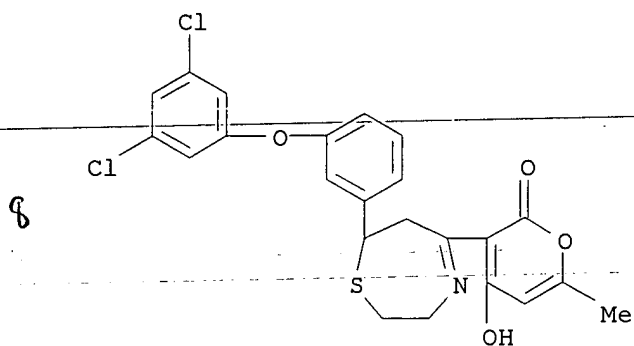
RN 369387-74-6 CAPLUS

CN 2H-Pyran-2-one, 3-[7-[3-(3,4-dichlorophenoxy)phenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



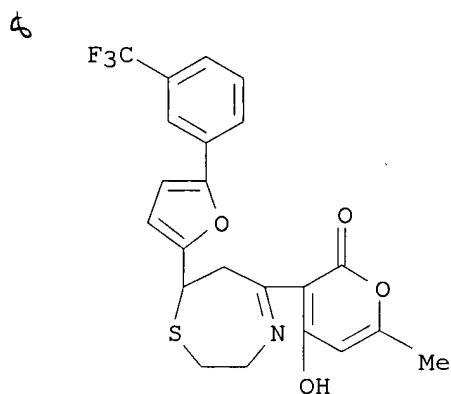
RN 369387-76-8 CAPLUS

CN 2H-Pyran-2-one, 3-[7-[3-(3,5-dichlorophenoxy)phenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



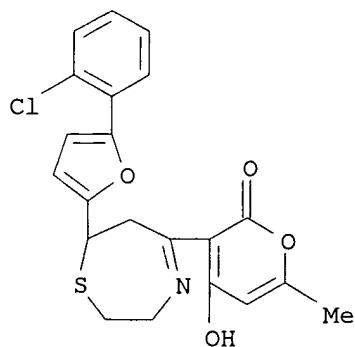
RN 369387-77-9 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[5-[3-(trifluoromethyl)phenyl]-2-furanyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



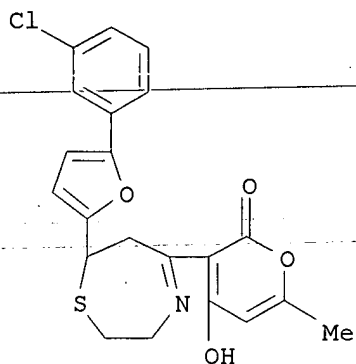
RN 369387-79-1 CAPLUS

CN 2H-Pyran-2-one, 3-[7-[5-(2-chlorophenyl)-2-furanyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



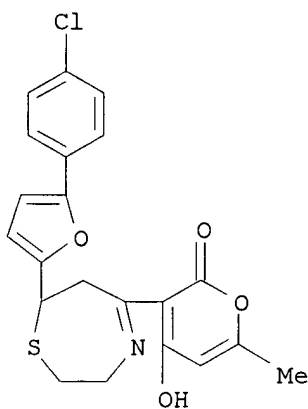
RN 369387-80-4 CAPLUS

CN 2H-Pyran-2-one, 3-[7-[5-(3-chlorophenyl)-2-furanyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



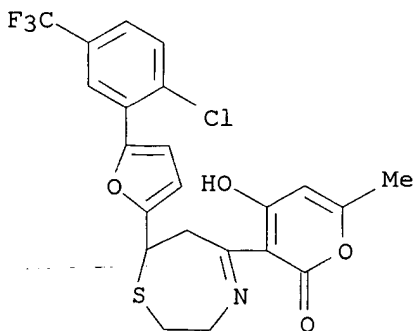
RN 369387-81-5 CAPLUS

CN 2H-Pyran-2-one, 3-[7-[5-(4-chlorophenyl)-2-furanyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 369387-82-6 CAPLUS

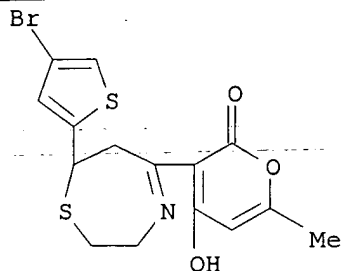
CN 2H-Pyran-2-one, 3-[7-[5-[2-chloro-5-(trifluoromethyl)phenyl]-2-furanyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



09/836,548

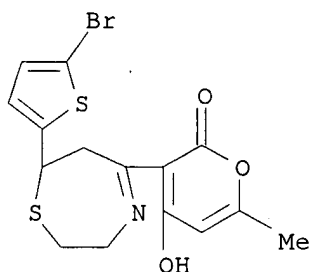
RN 369387-83-7 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(4-bromo-2-thienyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



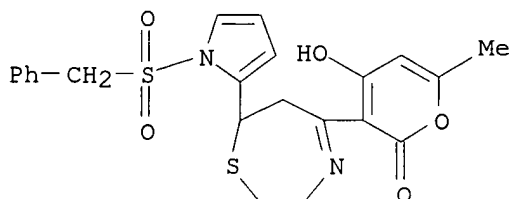
RN 369387-84-8 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(5-bromo-2-thienyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



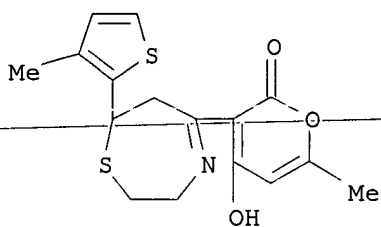
RN 369387-86-0 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[1-[(phenylmethyl)sulfonyl]-1H-pyrrol-2-yl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



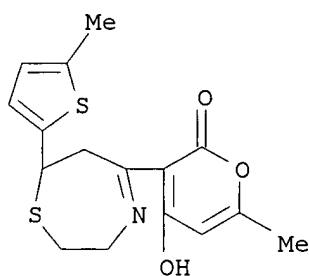
RN 369387-88-2 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3-methyl-2-thienyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



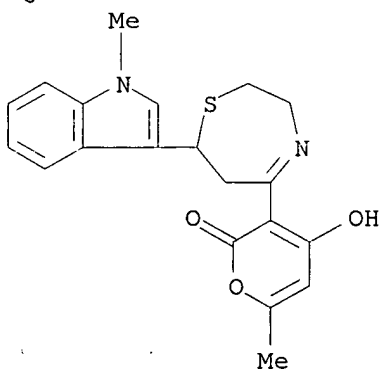
RN 369387-89-3 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(5-methyl-2-thienyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 369387-91-7 CAPLUS

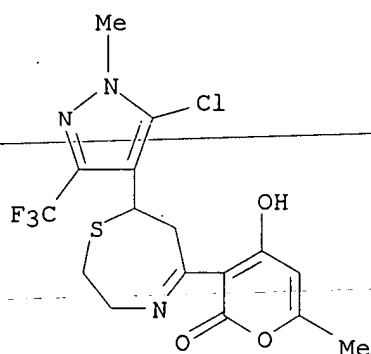
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(1-methyl-1H-indol-3-yl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 369387-93-9 CAPLUS

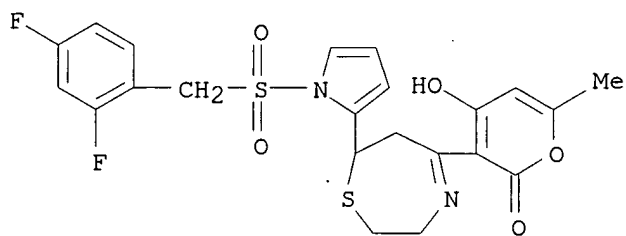
CN 2H-Pyran-2-one, 3-[7-[5-chloro-1-methyl-3-(trifluoromethyl)-1H-pyrazol-4-yl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)





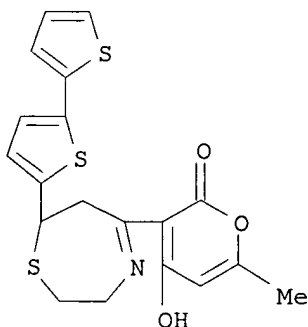
RN 369387-94-0 CAPLUS

CN 2H-Pyran-2-one, 3-[7-[1-[(2,4-difluorophenyl)methyl]sulfonyl]-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



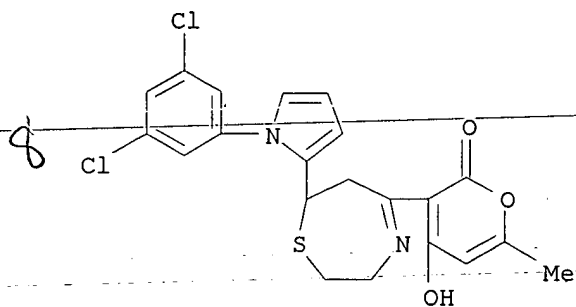
RN 369387-96-2 CAPLUS

CN 2H-Pyran-2-one, 3-[7-[2,2'-bithiophen]-5-yl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl)-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

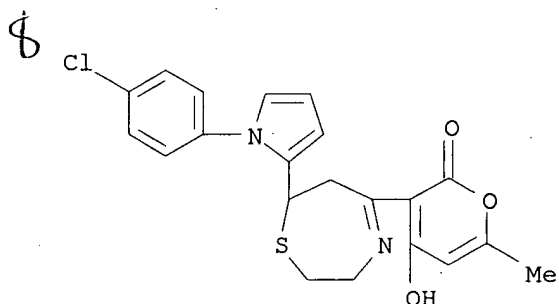


RN 369387-97-3 CAPLUS

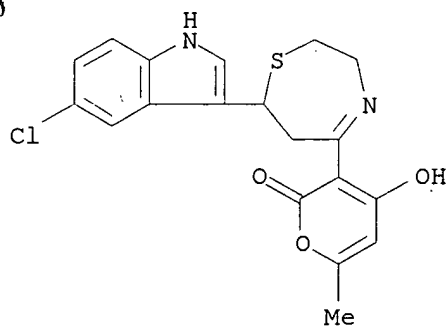
CN 2H-Pyran-2-one, 3-[7-[1-(3,5-dichlorophenyl)-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



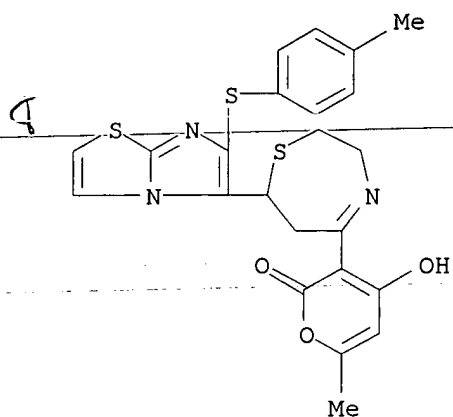
RN 369387-99-5 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-[1-(4-chlorophenyl)-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 369388-00-1 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-(5-chloro-1H-indol-3-yl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

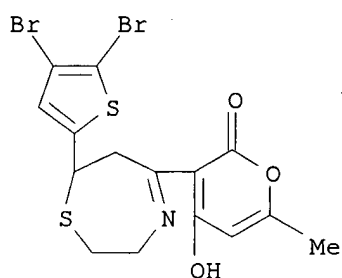


RN 369388-03-4 CAPLUS  
 CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[6-[(4-methylphenyl)thio]imidazo[2,1-b]thiazol-5-yl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



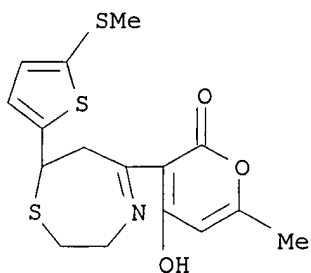
RN 369388-06-7 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(4,5-dibromo-2-thienyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



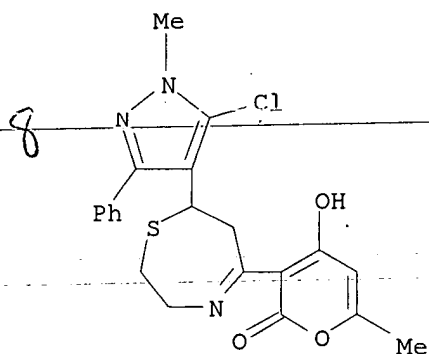
RN 369388-09-0 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[5-(methylthio)-2-thienyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



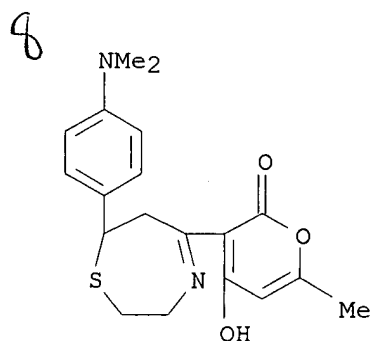
RN 369388-12-5 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(5-chloro-1-methyl-3-phenyl-1H-pyrazol-4-yl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



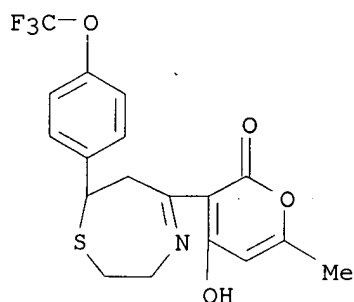
RN 369388-14-7 CAPLUS

CN 2H-Pyran-2-one, 3-[7-[4-(dimethylamino)phenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



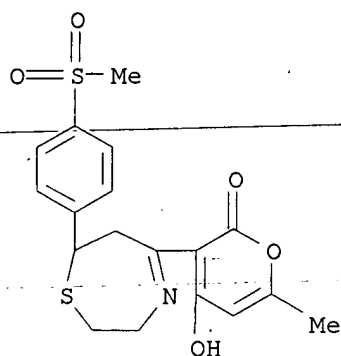
RN 369388-15-8 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-(trifluoromethoxy)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



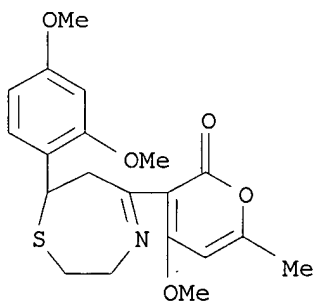
RN 369388-17-0 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-(methylsulfonyl)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



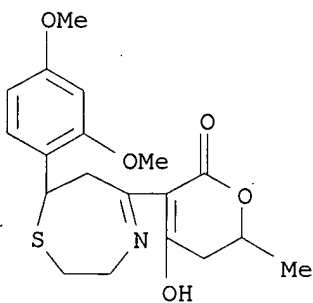
RN 369388-19-2 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-methoxy-6-methyl- (9CI) (CA INDEX NAME)



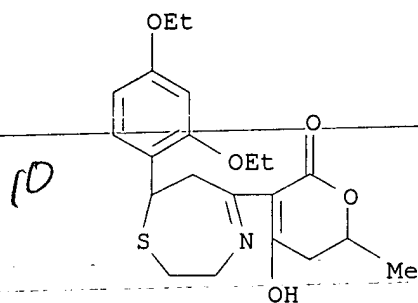
RN 369388-21-6 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-5,6-dihydro-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



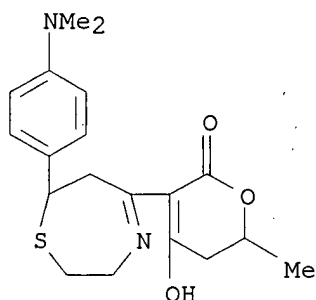
RN 369388-23-8 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,4-diethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-5,6-dihydro-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



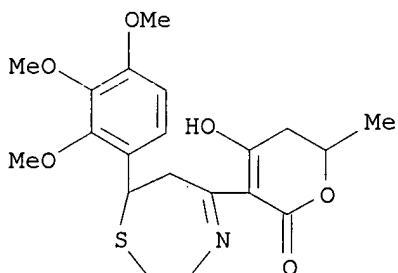
RN 369388-25-0 CAPLUS

CN 2H-Pyran-2-one, 3-[7-[4-(dimethylamino)phenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-5,6-dihydro-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



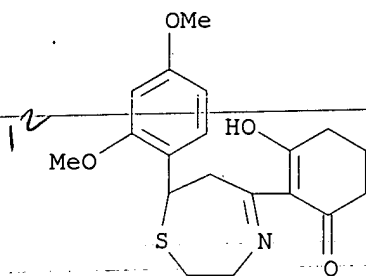
RN 369388-27-2 CAPLUS

CN 2H-Pyran-2-one, 5,6-dihydro-4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)

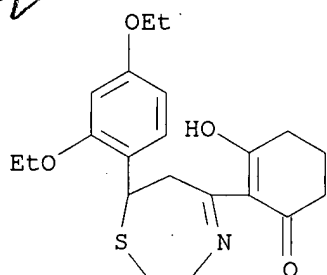


RN 369388-29-4 CAPLUS

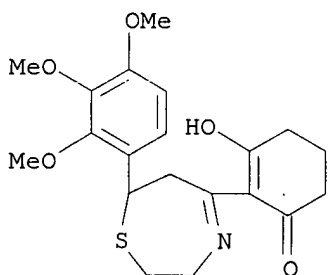
CN 2-Cyclohexen-1-one, 2-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-3-hydroxy- (9CI) (CA INDEX NAME)



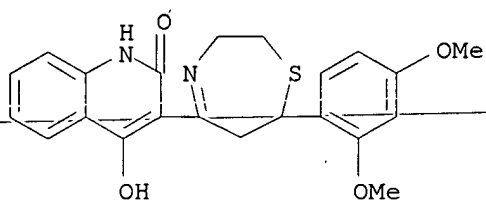
RN 369388-31-8 CAPLUS  
 CN 2-Cyclohexen-1-one, 2-[7-(2,4-diethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-3-hydroxy- (9CI) (CA INDEX NAME)



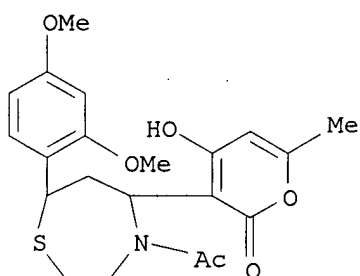
RN 369388-33-0 CAPLUS  
 CN 2-Cyclohexen-1-one, 3-hydroxy-2-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



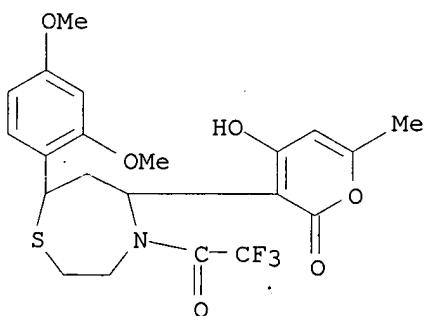
RN 369388-35-2 CAPLUS  
 CN 2(1H)-Quinolinone, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy- (9CI) (CA INDEX NAME)



RN 369388-44-3 CAPLUS  
 CN 1,4-Thiazepine, 4-acetyl-7-(2,4-dimethoxyphenyl)hexahydro-5-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)- (9CI) (CA INDEX NAME)

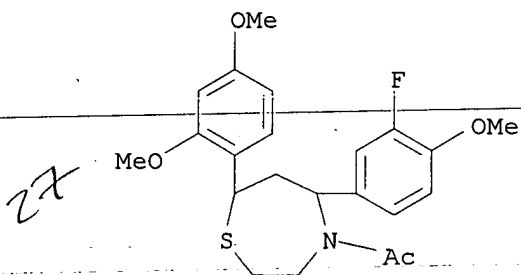


RN 369388-46-5 CAPLUS  
 CN 1,4-Thiazepine, 7-(2,4-dimethoxyphenyl)hexahydro-5-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)-4-(trifluoroacetyl)- (9CI) (CA INDEX NAME)

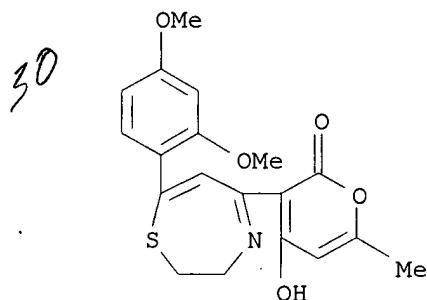


RN 369388-48-7 CAPLUS  
 CN 1,4-Thiazepine, 4-acetyl-7-(2,4-dimethoxyphenyl)-5-(3-fluoro-4-methoxyphenyl)hexahydro- (9CI) (CA INDEX NAME)

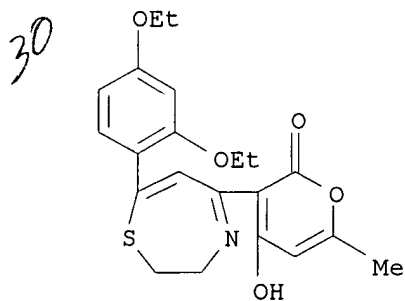




RN 369388-50-1 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3-dihydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

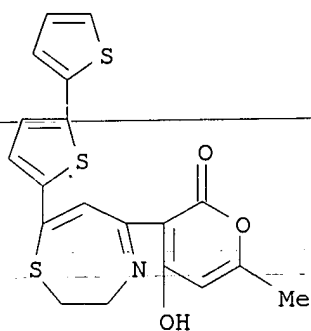


RN 369388-52-3 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-(2,4-diethoxyphenyl)-2,3-dihydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



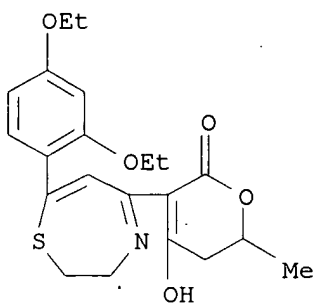
RN 369388-54-5 CAPLUS  
 CN 2H-Pyran-2-one, 3-(7-[2,2'-bithiophen]-5-yl)-2,3-dihydro-1,4-thiazepin-5-yl)-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

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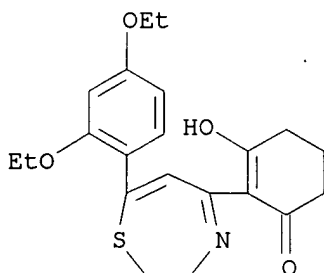
RN 369388-56-7 CAPLUS  
CN 2H-Pyran-2-one, 3-[7-(2,4-diethoxyphenyl)-2,3-dihydro-1,4-thiazepin-5-yl]-5,6-dihydro-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

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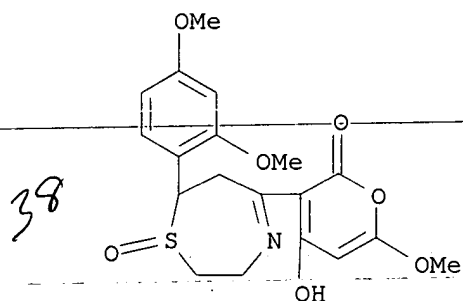


RN 369388-58-9 CAPLUS  
CN 2-Cyclohexen-1-one, 2-[7-(2,4-diethoxyphenyl)-2,3-dihydro-1,4-thiazepin-5-yl]-3-hydroxy- (9CI) (CA INDEX NAME)

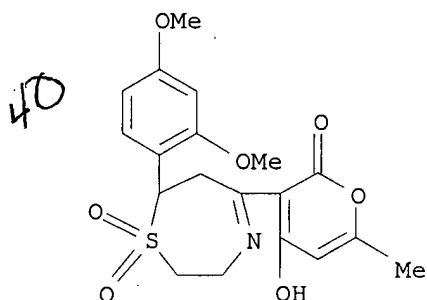
34



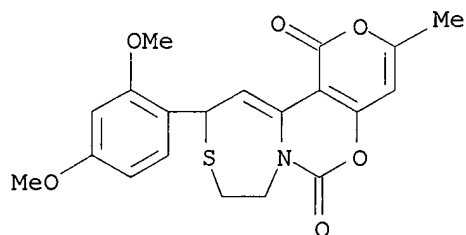
RN 369388-60-3 CAPLUS  
CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1-oxido-1,4-thiazepin-5-yl]-4-hydroxy-6-methoxy- (9CI) (CA INDEX NAME)



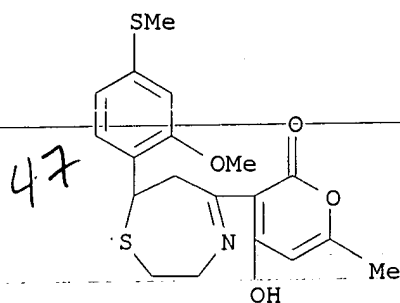
RN 369388-62-5 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,1-dioxido-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



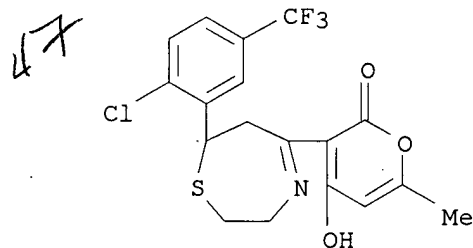
RN 369388-67-0 CAPLUS  
 CN 1H,6H,11H-Pyrano[3',4':5,6][1,3]oxazino[3,4-d][1,4]thiazepine-1,6-dione, 11-(2,4-dimethoxyphenyl)-8,9-dihydro-3-methyl- (9CI) (CA INDEX NAME)



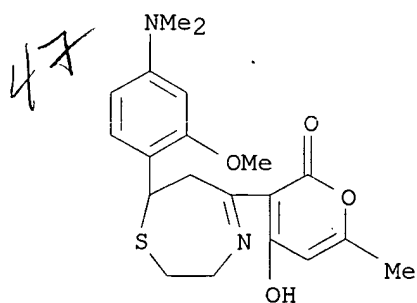
RN 369388-69-2 CAPLUS  
 CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[2-methoxy-4-(methylthio)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



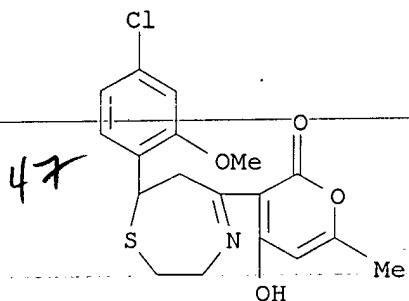
RN 369388-71-6 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-[2-chloro-5-(trifluoromethyl)phenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



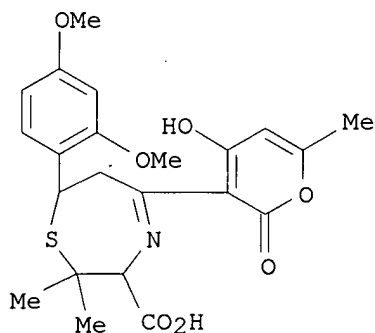
RN 369388-73-8 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-[4-(dimethylamino)-2-methoxyphenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 369388-75-0 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-(4-chloro-2-methoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

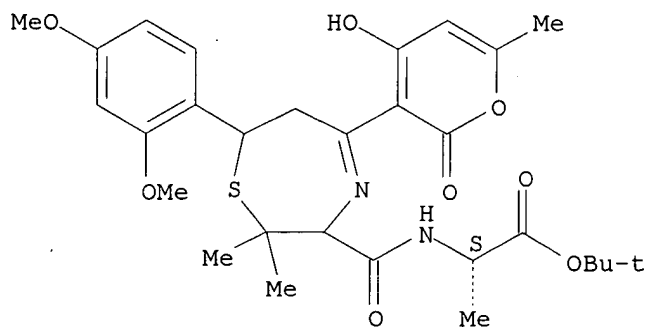


RN 369388-79-4 CAPLUS  
 CN 1,4-Thiazepine-3-carboxylic acid, 7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-5-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)-2,2-dimethyl- (9CI)  
 (CA INDEX NAME)

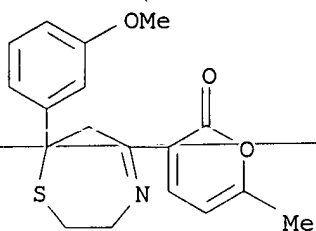


RN 369388-81-8 CAPLUS  
 CN L-Alanine, N-[[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-5-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)-2,2-dimethyl-1,4-thiazepin-3-yl]carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

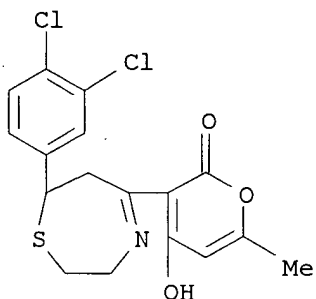
Absolute stereochemistry.



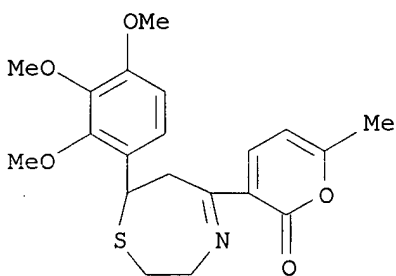
RN 369388-85-2 CAPLUS  
 CN 2H-Pyran-2-one, 6-methyl-3-[2,3,6,7-tetrahydro-7-(3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



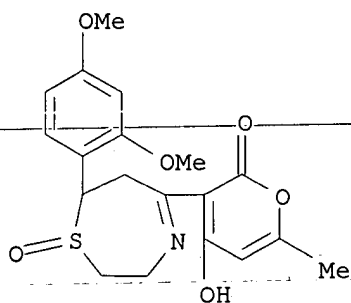
RN 369388-89-6 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-(3,4-dichlorophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 369388-91-0 CAPLUS  
 CN 2H-Pyran-2-one, 6-methyl-3-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)

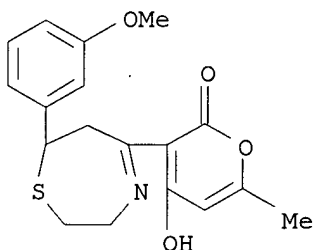


RN 369389-71-9 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1-oxido-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



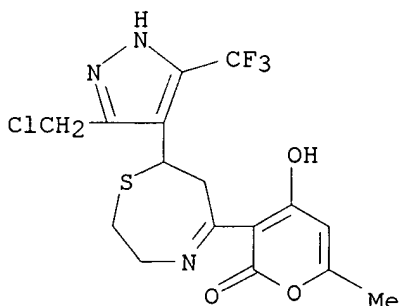
RN 369389-72-0 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 369605-23-2 CAPLUS

CN 2H-Pyran-2-one, 3-[7-[3-(chloromethyl)-5-(trifluoromethyl)-1H-pyrazol-4-yl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



IT 369389-06-0, 7-(2,4-Dimethoxyphenyl)-5-(3-fluoro-4-methoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepine

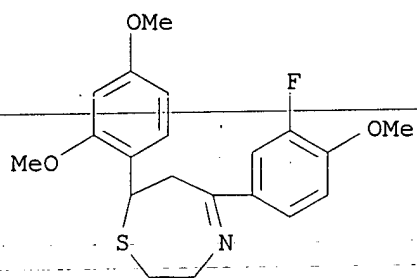
RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant; prepn. of substituted 1,4-thiazepines and analogs as activators of caspases and inducers of apoptosis for treatment of cancer and other proliferative diseases)

RN 369389-06-0 CAPLUS

CN 1,4-Thiazepine, 7-(2,4-dimethoxyphenyl)-5-(3-fluoro-4-methoxyphenyl)-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)

09/836,548





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ACCESSION NUMBER: 2001:617988 CAPLUS

DOCUMENT NUMBER: 135:195581

TITLE: Preparation of thiazepinyl hydroxamic acid derivatives as matrix metalloproteinase inhibitors

INVENTOR(S): Neya, Masahiro; Yamazaki, Hitoshi; Ohne, Kazuhiko; Sawada, Yuki; Mizutani, Tsuyoshi; Imamura, Yoshimasa; Mukai, Noriko

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 446 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

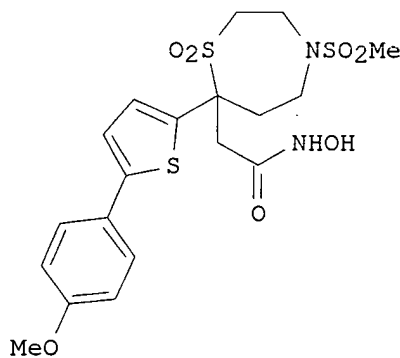
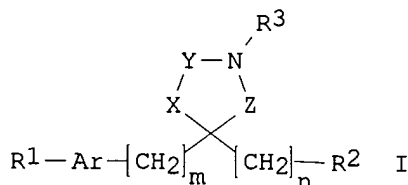
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001060808	A1	20010823	WO 2001-JP1206	20010220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: AU 2000-5751 A 20000221  
AU 2000-8603 A 20000706

OTHER SOURCE(S): MARPAT 135:195581

GI



AB The title compds. [I; R<sub>1</sub> = halo, alkoxy, (un)substituted aryl, etc.; R<sub>2</sub> = amidated carboxy; R<sub>3</sub> = H, acyl; Ar = aryl, heterocyclyl; X = S, SO, SO<sub>2</sub>; Y, Z = alkylene; m, n = 0-2], useful as inhibitors of matrix metalloproteinases (MMP) or the prodn. of tumor necrosis factor .alpha. (TNF .alpha.), were prep'd. E.g., a multi-step synthesis of II which showed IC<sub>50</sub> of 2.85 nM against human MMP-9, was given.

09/836,548

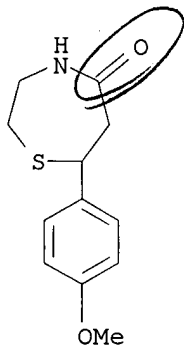
IT 73920-60-2P 355849-35-3P 355849-50-2P  
355850-10-1P 355850-16-7P 355850-22-5P  
355850-62-3P 355850-82-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(prepn. of thiazepinyl hydroxamic acid derivs. as matrix  
metalloproteinase inhibitors)

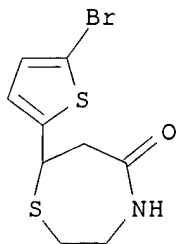
RN 73920-60-2 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(4-methoxyphenyl)- (9CI) (CA INDEX  
NAME)



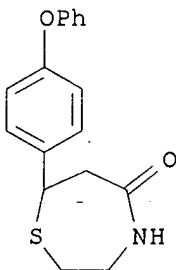
RN 355849-35-3 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, 7-(5-bromo-2-thienyl)tetrahydro- (9CI) (CA INDEX  
NAME)



RN 355849-50-2 CAPLUS

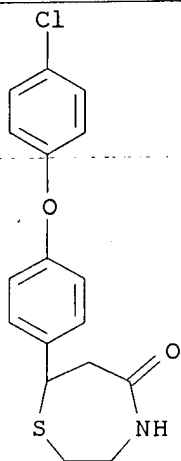
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(4-phenoxyphenyl)- (9CI) (CA INDEX  
NAME)



09/836,548

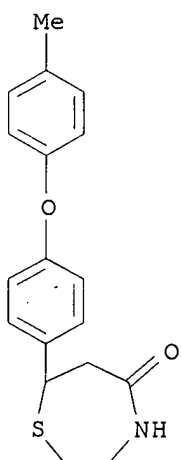
RN 355850-10-1 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, 7-[4-(4-chlorophenoxy)phenyl]tetrahydro- (9CI)  
(CA INDEX NAME)



RN 355850-16-7 CAPLUS

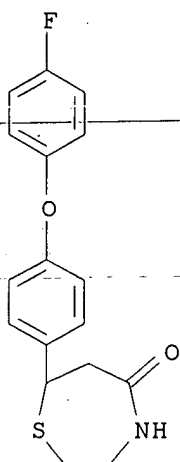
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-[4-(4-methylphenoxy)phenyl]- (9CI)  
(CA INDEX NAME)



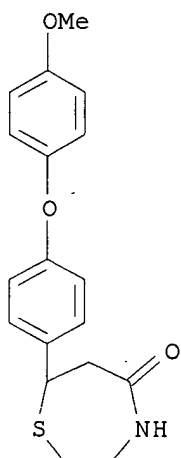
RN 355850-22-5 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, 7-[4-(4-fluorophenoxy)phenyl]tetrahydro- (9CI)  
(CA INDEX NAME)

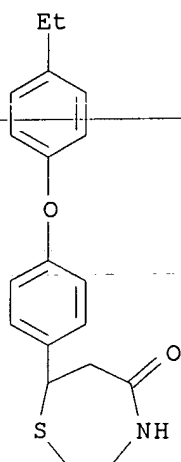
09/836,548



RN 355850-62-3 CAPLUS  
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-[4-(4-methoxyphenoxy)phenyl]- (9CI)  
(CA INDEX NAME)



RN 355850-82-7 CAPLUS  
CN 1,4-Thiazepin-5(2H)-one, 7-[4-(4-ethylphenoxy)phenyl]tetrahydro- (9CI)  
(CA INDEX NAME)



REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 5 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:258482 CAPLUS

DOCUMENT NUMBER: 133:117069

TITLE: Dissecting cellular processes using small molecules:  
identification of colchicine-like, taxol-like and  
other small molecules that perturb mitosisAUTHOR(S): Haggarty, Stephen J.; Mayer, Thomas U.; Miyamoto,  
David T.; Fathi, Reza; King, Randall W.; Mitchison,  
Timothy J.; Schreiber, Stuart L.CORPORATE SOURCE: Harvard Institute of Chemistry and Cell Biology,  
Harvard Medical School, Boston, MA, 02115, USASOURCE: Chemistry & Biology (2000), 7(4), 275-286  
CODEN: CBOLE2; ISSN: 1074-5521

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

April

AB Background: Understanding the mol. mechanisms of complex cellular processes requires unbiased means to identify and to alter conditionally gene products that function in a pathway of interest. Although random mutagenesis and screening (forward genetics) provide a useful means to this end, the complexity of the genome, long generation time and redundancy of gene function have limited their use with mammalian systems. We sought to develop an analogous process using small mols. to modulate conditionally the function of proteins. We hoped to identify simultaneously small mols. that may serve as leads for the development of therapeutically useful agents. Results: We report the results of a high-throughput, phenotype-based screen for identifying cell-permeable small mols. that affect mitosis of mammalian cells. The predominant class of compds. that emerged directly alters the stability of microtubules in the mitotic spindle. Although many of these compds. show the colchicine-like property of destabilizing microtubules, one member shows the taxol-like property of stabilizing microtubules. Another class of compds. alters chromosome segregation by novel mechanisms that do not involve direct interactions with microtubules. Conclusions: The identification of structurally diverse small mols. that affect the mammalian mitotic machinery from a large library of synthetic compds. illustrates the use of chem. genetics in dissecting an essential cellular pathway. This screen identified five compds. that affect mitosis without directly targeting microtubules. Understanding the mechanism of action of these compds., along with future screening efforts, promises to help elucidate the mol. mechanisms involved in chromosome segregation during mitosis.

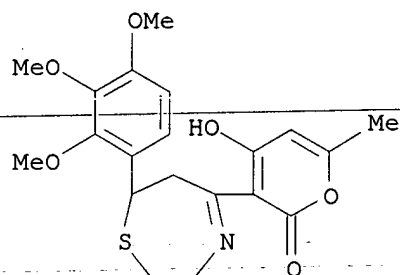
IT 257292-28-7 257292-29-8 257292-30-1  
257292-31-2 257292-32-3 257292-33-4  
257292-34-5 257292-35-6 257292-36-7  
257292-37-8 257292-38-9 257292-39-0  
257292-40-3 257292-41-4 257292-42-5  
257292-43-6 257292-44-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(phenotype-based screening of compd. library to identify cell-permeable small mols. that affect mitosis of mammalian cells)

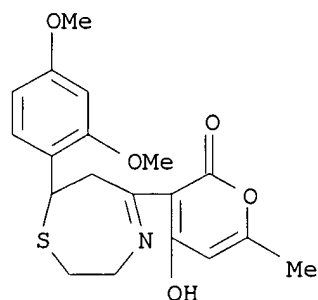
RN 257292-28-7 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



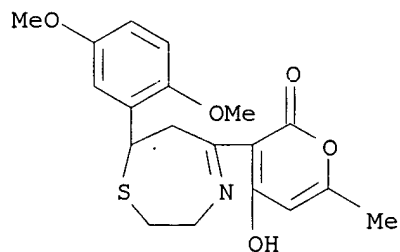
RN 257292-29-8 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



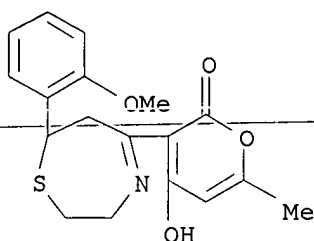
RN 257292-30-1 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,5-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



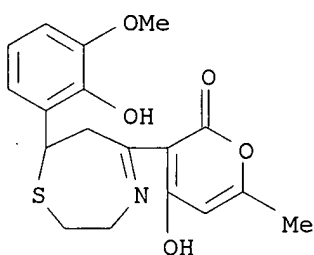
RN 257292-31-2 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



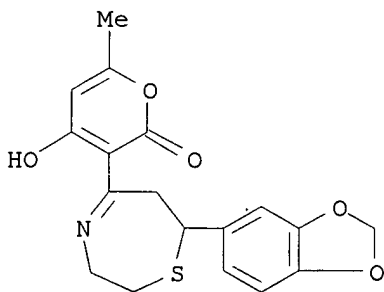
RN 257292-32-3 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2-hydroxy-3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 257292-33-4 CAPLUS

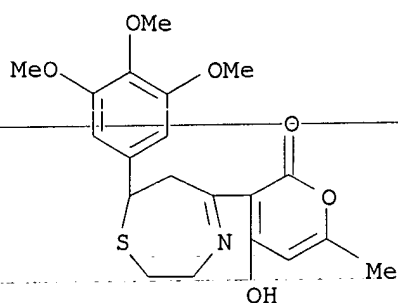
CN 2H-Pyran-2-one, 3-[7-(1,3-benzodioxol-5-yl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 257292-34-5 CAPLUS

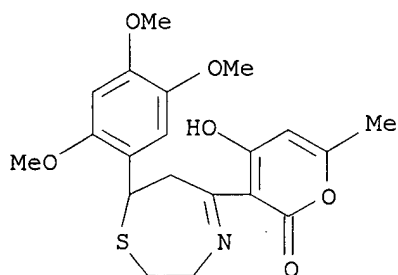
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3,4,5-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)





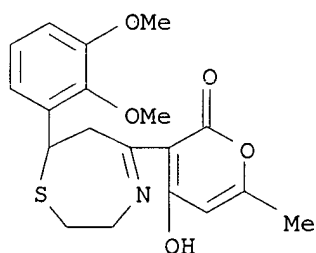
RN 257292-35-6 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,4,5-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



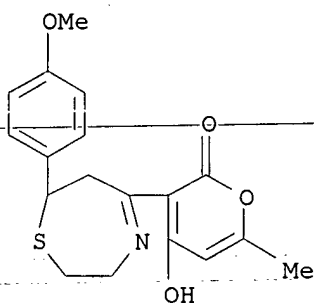
RN 257292-36-7 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,3-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



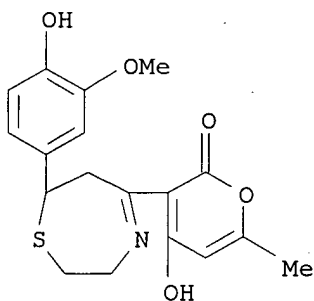
RN 257292-37-8 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



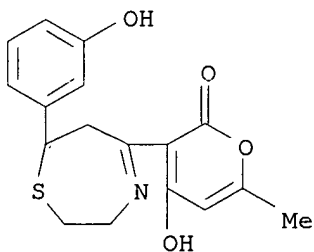
RN 257292-38-9 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-hydroxy-3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 257292-39-0 CAPLUS

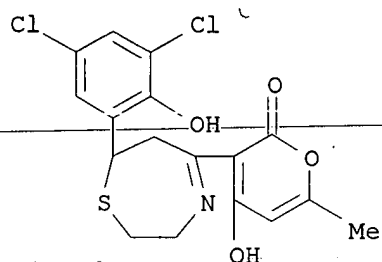
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3-hydroxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



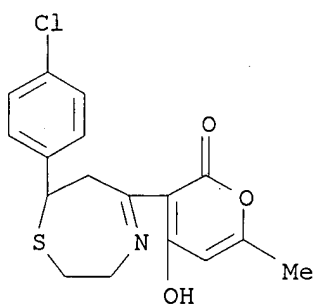
RN 257292-40-3 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(3,5-dichloro-2-hydroxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

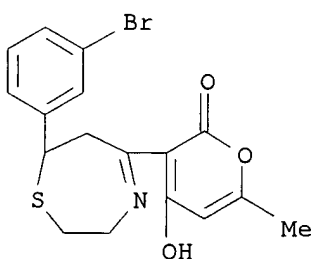
09/836,548



RN 257292-41-4 CAPLUS  
CN 2H-Pyran-2-one, 3-[7-(4-chlorophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

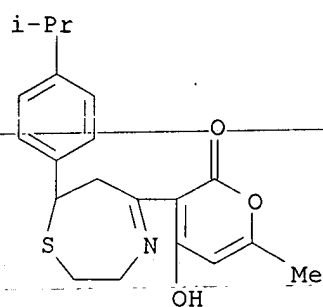


RN 257292-42-5 CAPLUS  
CN 2H-Pyran-2-one, 3-[7-(3-bromophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



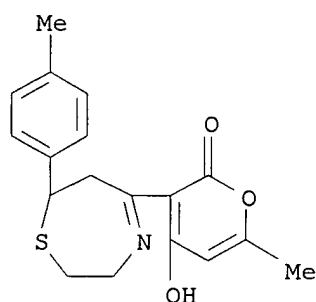
RN 257292-43-6 CAPLUS  
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-(1-methylethyl)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)

09/836,548



RN 257292-44-7 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-methylphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

35

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

09/836,548

113 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:148732 CAPLUS

DOCUMENT NUMBER: 132:293716

TITLE: Tetrahydrothiapyran-4-ones. Source for annelated 1,2,3-selena/thiadiazoles and their reactivity

AUTHOR(S): Reddy, D. Bhaskar; Reddy, A. Somasekhar; Reddy, N. Subba

CORPORATE SOURCE: Department of Chemistry, Sri Venkateswara University, Tirupati, 517 502, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1999), 38B(12), 1342-1348

CODEN: IJSBDB; ISSN: 0376-4699

PUBLISHER: National Institute of Science Communication, CSIR

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:293716

AB 1,2,3-Selenadiazole and 1,2,3-thiadiazole rings were fused to 2,6-diaryl-(3-alkyl)-tetrahydrothiapyran-4-ones (I) utilizing an .alpha.-keto methylene group by reaction of the corresponding semicarbazones with SOCl<sub>2</sub> or SeO<sub>2</sub>. The reactivity of I was also studied viz., Beckmann rearrangement, Shapiro reaction, Strecker synthesis of .alpha.-amino acids, etc.

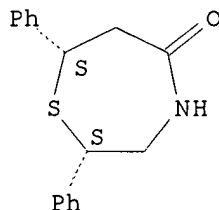
IT 264129-41-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of annelated selenadiazoles and thiadiazoles from hydrothiapyranones.)

RN 264129-41-1 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-2,7-diphenyl-, (2R,7R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

19

THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:98918 CAPLUS

DOCUMENT NUMBER: 132:148734

TITLE: Method and device for high-throughput screening of molecules and compounds for their effects on biological and chemical processes

INVENTOR(S): Stockwell, Brent R.; Schreiber, Stuart L.; Haggarty, Stephen J.; Mitchison, Timothy J.; Kapoor, Tarun M.; Mayer, Thomas

PATENT ASSIGNEE(S): President and Fellows of Harvard College, USA

SOURCE: PCT-Int. Appl., 153 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000007017	A2	20000210	WO 1999-US17046	19990727
WO 2000007017	A3	20000504		
W: AU, CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9953223	A1	20000221	AU 1999-53223	19990727
PRIORITY APPLN. INFO.:			US 1998-94305P	P 19980727
			US 1999-131765P	P 19990430
			US 1999-137039P	P 19990601
			WO 1999-US17046	W 19990727

OTHER SOURCE(S): MARPAT 132:148734

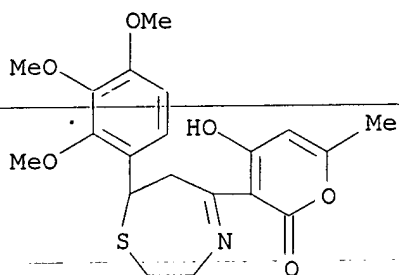
AB The present invention provides a system for high-throughput anal. of chem. compds. Assays are performed in a high d. platform, and compds. having pre-detd. desirable effects are identified. Preferably, the compds. have biol. effects, more preferably, the assays and detection are performed on whole cells. The system has a high-d. array of at least 100 reaction vessels, each vessel having a small vol. A 384-well 5-bromodeoxyuridine cyto blot assay was used to detect changes in DNA synthesis in mink lung cells caused by various agents.

IT 257292-28-7 257292-29-8 257292-30-1  
 257292-31-2 257292-32-3 257292-33-4  
 257292-34-5 257292-35-6 257292-36-7  
 257292-37-8 257292-38-9 257292-39-0  
 257292-40-3 257292-41-4 257292-42-5  
 257292-43-6 257292-44-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
 (microtubules destabilization by; method and device for high-throughput screening of mols. and compds. for their effects on biol. and chem. processes)

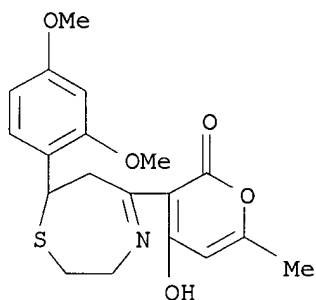
RN 257292-28-7 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



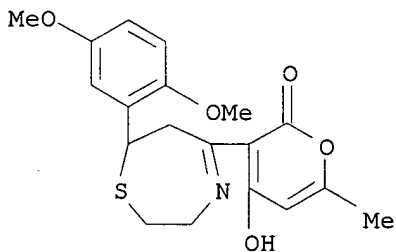
RN 257292-29-8 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



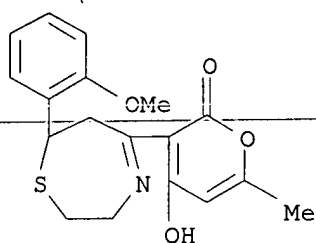
RN 257292-30-1 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,5-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



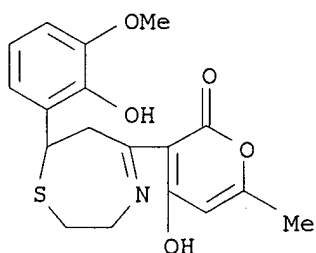
RN 257292-31-2 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



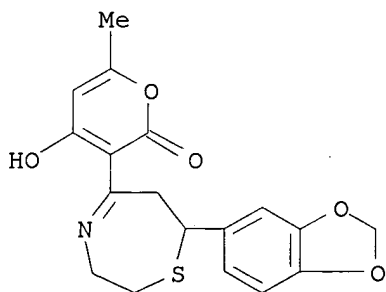
RN 257292-32-3 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2-hydroxy-3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 257292-33-4 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(1,3-benzodioxol-5-yl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

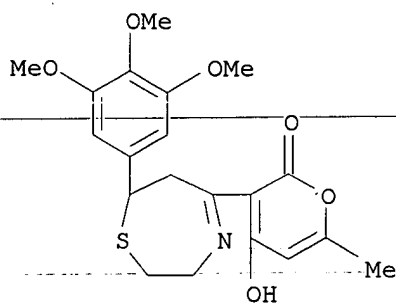


RN 257292-34-5 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3,4,5-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)

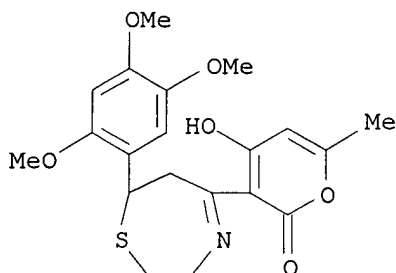


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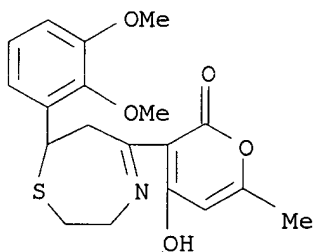
RN 257292-35-6 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,4,5-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



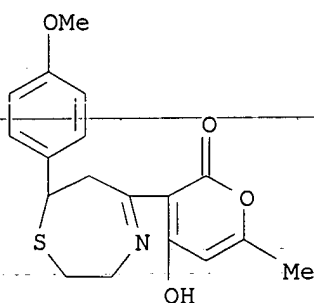
RN 257292-36-7 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,3-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



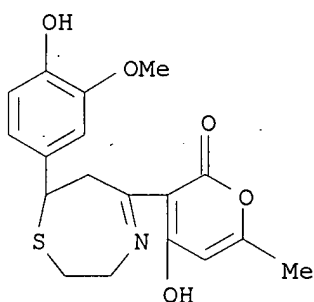
RN 257292-37-8 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



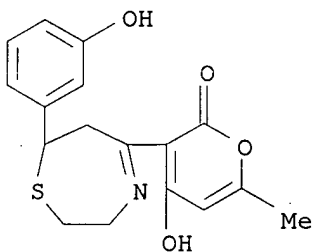
RN 257292-38-9 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-hydroxy-3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



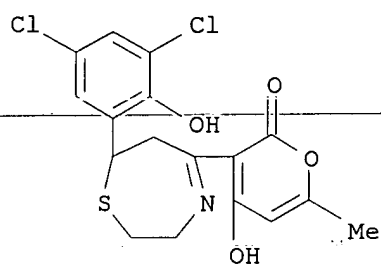
RN 257292-39-0 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3-hydroxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)

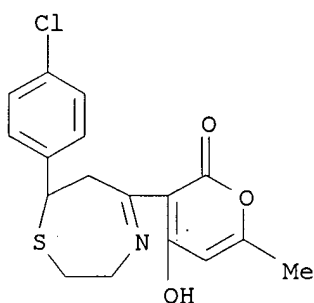


RN 257292-40-3 CAPLUS

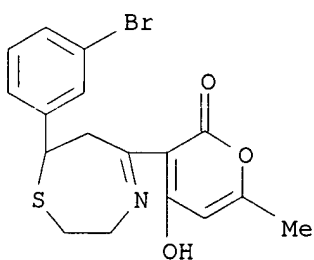
CN 2H-Pyran-2-one, 3-[7-(3,5-dichloro-2-hydroxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 257292-41-4 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-(4-chlorophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

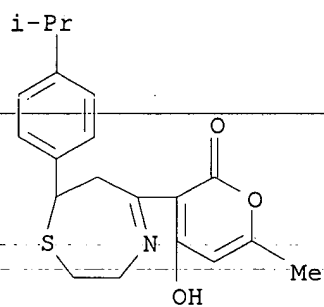


RN 257292-42-5 CAPLUS  
 CN 2H-Pyran-2-one, 3-[7-(3-bromophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



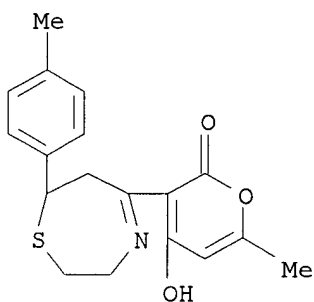
RN 257292-43-6 CAPLUS  
 CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-(1-methylethyl)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)

09/836,548



RN 257292-44-7 CAPLUS

CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-methylphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



09/836,548

~~LI3~~ ANSWER 8 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:245026 CAPLUS

DOCUMENT NUMBER: 120:245026

TITLE: Synthesis of 2,4-diaryl-3-(arylsulfonyl)-2,3-dihydro-1,5-benzothiazepines

AUTHOR(S): Reddey, D. Bhaskar; Sankaraiah, B.; Reddy, S.; Reddy, N. Subba; Reddy, P. V. Ramana

CORPORATE SOURCE: Dep. Chem., Sri Venkateswara Univ., Tirupati, 517 502, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1993), 32B(11), 1165-7

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The reaction of 2-aminothiophenol with 1,3-diaryl-2-(arylsulfonyl)-2-propen-1-ones I (R1 = H, R2 = H, 4-Cl, 4-Br; R1 = 4-Cl, R2 = 4-Br; R1 = 4-Me, 4-Cl, R2 = H) in dry toluene at reflux temp. affords a mixt. of 1,3-diaryl-2-(arylsulfonyl)-3-(2'-aminophenylmercapto)-1-ones II and 2,4-diaryl-3-(arylsulfonyl)-2,3-dihydro-1,5-benzothiazepines III. The dehydrative cyclization of II yields III. The structures of II and III have been established by spectral data.

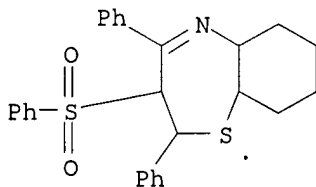
IT 154324-21-7P 154324-22-8P 154324-23-9P

154324-24-0P 154324-25-1P 154324-26-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

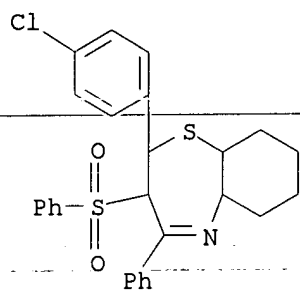
RN 154324-21-7 CAPLUS

CN 1,5-Benzothiazepine, 2,3,5a,6,7,8,9,9a-octahydro-2,4-diphenyl-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



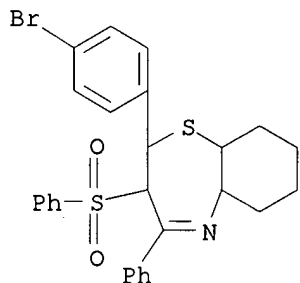
RN 154324-22-8 CAPLUS

CN 1,5-Benzothiazepine, 2-(4-chlorophenyl)-2,3,5a,6,7,8,9,9a-octahydro-4-phenyl-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



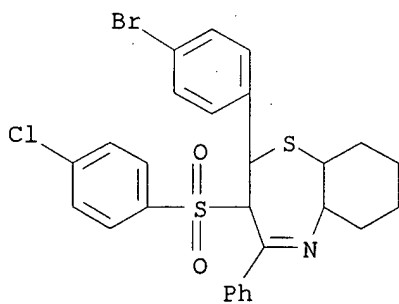
RN 154324-23-9 CAPLUS

CN 1,5-Benzothiazepine, 2-(4-bromophenyl)-2,3,5a,6,7,8,9,9a-octahydro-4-phenyl-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



RN 154324-24-0 CAPLUS

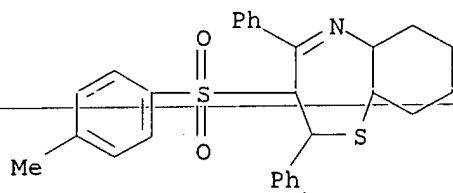
CN 1,5-Benzothiazepine, 2-(4-bromophenyl)-3-[(4-chlorophenyl)sulfonyl]-2,3,5a,6,7,8,9,9a-octahydro-4-phenyl- (9CI) (CA INDEX NAME)



RN 154324-25-1 CAPLUS

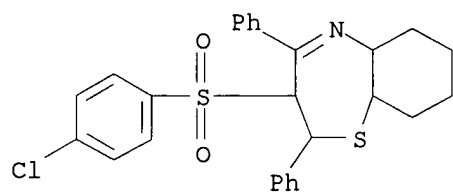
CN 1,5-Benzothiazepine, 2,3,5a,6,7,8,9,9a-octahydro-3-[(4-methylphenyl)sulfonyl]-2,4-diphenyl- (9CI) (CA INDEX NAME)

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RN 154324-26-2 CAPLUS

CN 1,5-Benzothiazepine, 3-[(4-chlorophenyl)sulfonyl]-2,3,5a,6,7,8,9,9a-octahydro-2,4-diphenyl- (9CI) (CA INDEX NAME)



~~143~~ ANSWER 9 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:539162 CAPLUS

DOCUMENT NUMBER: 119:139162

TITLE: Synthesis, antiparasitic and antifungal activities of arylalkyl and arylvinylthiazolines

AUTHOR(S): Caujolle, R.; Baziard-Mouysset, G.; Favrot, J. D.; Payard, M.; Loiseau, P. R.; Amarouch, H.; Linas, M. D.; Seguela, J. P.; Loiseau, P. M.; et al.

CORPORATE SOURCE: Dep. Chim., Fac. Pharm., Toulouse, 31000, Fr.

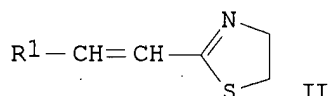
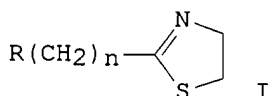
SOURCE: European Journal of Medicinal Chemistry (1993), 28(1); 29-35

CODEN: EJMCA5; ISSN: 0223-5234

DOCUMENT TYPE: Journal

LANGUAGE: French

GI



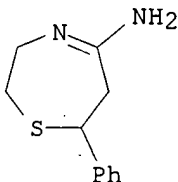
AB Twenty-seven arylalkyl- [I; R = Ph, n = 1, 2; R = 4-MeC6H4, 4-MeOC6H4, 3,4-(MeO)2C6H3, 4-ClC6H4, 4-O2NC6H4, 2-thienyl, 1-, 2-naphthyl, n = 1] or arylvinylthiazolines [II; R1 = Ph, 4-MeC6H4, 4-MeOC6H4, 4-MeSC6H4, 3,4-(MeO)2C6H3, 3,4-(OCH2O)C6H3, 4-ClC6H4, 2,4-Cl2C6H3, 4-O2NC6H4, 2-thienyl, 2-furyl, 2-, 3-, 4-pyridyl, 2-naphthyl, 2-benzofuryl, 2-(4-benzopyranyl)] were synthesized and tested in vitro against three genera of nematodes, various yeasts and opportunistic fungi. Vinyl compds. II seem to have an interesting filaricidal activity against Molinema dessetae and antifungal activity against yeasts.

IT 149770-59-2P 149770-60-5P 149770-61-6P  
149770-62-7P 149770-63-8P 149770-64-9P  
149770-65-0P 149770-66-1P 149770-67-2P  
149770-68-3P 149770-69-4P 149770-70-7P  
149770-71-8P 149770-72-9P 149770-73-0P  
149770-74-1P 149770-75-2P

RL: SPN (Synthetic preparation); PREP. (Preparation)  
(prepn. of)

RN 149770-59-2 CAPLUS

CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-phenyl- (9CI) (CA INDEX NAME)



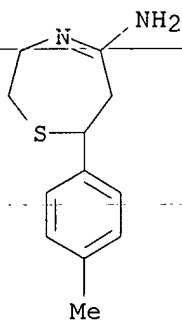
RN 149770-60-5 CAPLUS

CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(4-methylphenyl)- (9CI) (CA



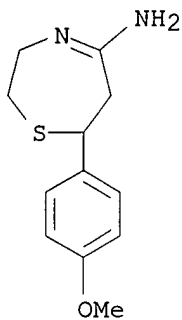
09/836,548

INDEX NAME)



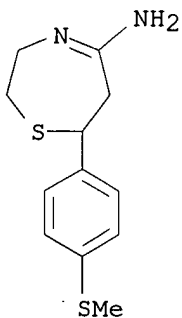
RN 149770-61-6 CAPLUS

CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 149770-62-7 CAPLUS

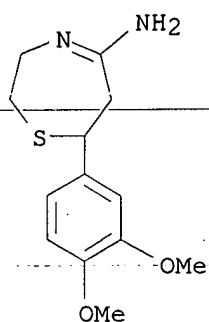
CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-[4-(methylthio)phenyl]- (9CI) (CA INDEX NAME)



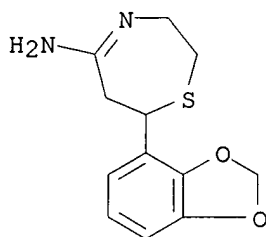
RN 149770-63-8 CAPLUS

CN 1,4-Thiazepin-5-amine, 7-(3,4-dimethoxyphenyl)-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)

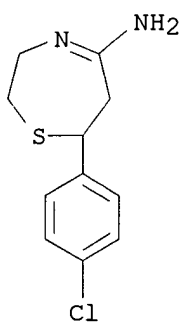
09/836,548



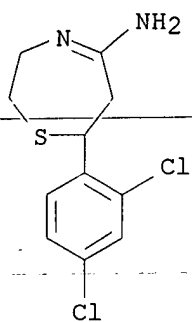
RN 149770-64-9 CAPLUS  
CN 1,4-Thiazepin-5-amine, 7-(1,3-benzodioxol-4-yl)-2,3,6,7-tetrahydro- (9CI)  
(CA INDEX NAME)



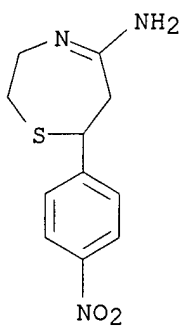
RN 149770-65-0 CAPLUS  
CN 1,4-Thiazepin-5-amine, 7-(4-chlorophenyl)-2,3,6,7-tetrahydro- (9CI) (CA  
INDEX NAME)



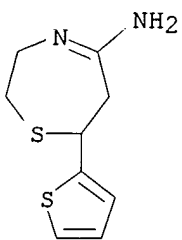
RN 149770-66-1 CAPLUS  
CN 1,4-Thiazepin-5-amine, 7-(2,4-dichlorophenyl)-2,3,6,7-tetrahydro- (9CI)  
(CA INDEX NAME)



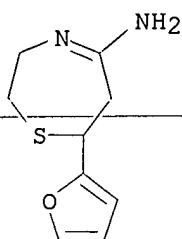
RN 149770-67-2 CAPLUS  
 CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



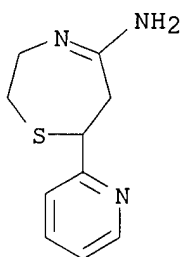
RN 149770-68-3 CAPLUS  
 CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(2-thienyl)- (9CI) (CA INDEX NAME)



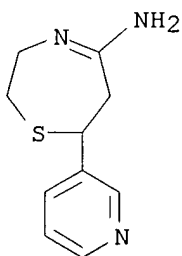
RN 149770-69-4 CAPLUS  
 CN 1,4-Thiazepin-5-amine, 7-(2-furanyl)-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)



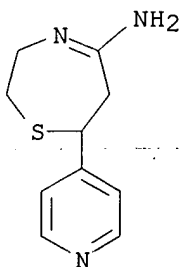
RN 149770-70-7 CAPLUS  
 CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(2-pyridinyl)- (9CI) (CA  
 INDEX NAME)



RN 149770-71-8 CAPLUS  
 CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(3-pyridinyl)- (9CI) (CA  
 INDEX NAME)



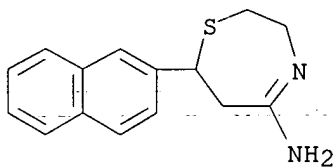
RN 149770-72-9 CAPLUS  
 CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(4-pyridinyl)- (9CI) (CA  
 INDEX NAME)



09/836,548

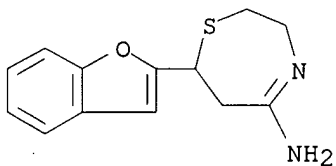
RN 149770-73-0 CAPLUS

CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(2-naphthalenyl)- (9CI) (CA INDEX NAME)



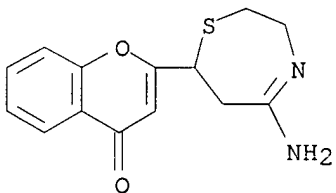
RN 149770-74-1 CAPLUS

CN 1,4-Thiazepin-5-amine, 7-(2-benzofuranyl)-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)



RN 149770-75-2 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(5-amino-2,3,6,7-tetrahydro-1,4-thiazepin-7-yl)- (9CI) (CA INDEX NAME)



~~DIS~~ ANSWER 10 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:449417 CAPLUS

DOCUMENT NUMBER: 119:49417

TITLE: Preparation of substituted thiazepines as central nervous system agents

INVENTOR(S): Smith, William John; Wise, Lawrence David; Wustrow, David Juergen

PATENT ASSIGNEE(S): Warner-Lambert Co., USA

SOURCE: PCT Int. Appl., 47 pp.

CODEN: PIXXD2

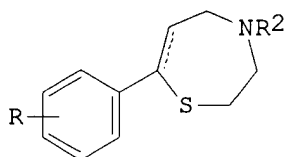
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9304053	A1	19930304	WO 1992-US6415	19920803
W: AU, CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE				
US 5206233	A	19930427	US 1991-750667	19910827
AU 9224370	A1	19930316	AU 1992-24370	19920803
PRIORITY APPLN. INFO.:			US 1991-750667	19910827
			WO 1992-US6415	19920803
OTHER SOURCE(S):		MARPAT 119:49417		
GI				



AB Title compds. I [R = H, alkyl, alkoxy, HO, halo, H<sub>2</sub>N, O<sub>2</sub>N, F<sub>3</sub>C, NC; R<sub>2</sub> = H, alkyl, R<sub>3</sub>(CH<sub>2</sub>)<sub>n</sub>, R<sub>3</sub>CO(CH<sub>2</sub>)<sub>n</sub>-1 wherein R<sub>3</sub> = pyridyl, cycloalkyl, n = 1-5], isomers and a salt thereof, are prepd. I showed antipsychotic activity. H<sub>2</sub>MCH<sub>2</sub>CH<sub>2</sub>SH.cntdot.HCl, MeOH, NaOH and Me trans-4-methoxycinnamate were reacted to give tetrahydro-7-(4-methoxyphenyl)-1,4-thiazepin-5-one which was treated with LiAlH<sub>4</sub> and AlCl<sub>3</sub> to give hexahydro-7-(4-methoxyphenyl)-1,4-thiazepine converted to HCl salt. Addnl. I were prepd.

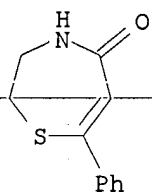
IT **65922-92-1P 73920-60-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

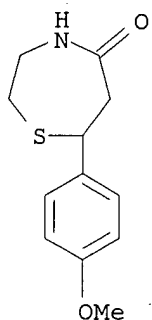
(prepn. and reaction of, in prepn. of central nervous system agents)

RN 65922-92-1 CAPLUS

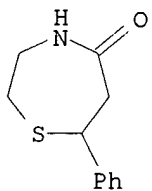
CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-7-phenyl- (9CI) (CA INDEX NAME)



RN 73920-60-2 CAPLUS  
 CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT 2897-03-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, prepn. of thiazepine central nervous system agents)  
 RN 2897-03-2 CAPLUS  
 CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



09/836,548

123 ANSWER 11 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:426532 CAPLUS

DOCUMENT NUMBER: 117:26532

TITLE: Synthesis, stereochemistry and pharmacological activity of rac-cis-tetrahydro-6-hydroxy-7-(4-methoxyphenyl)-1,4-thiazepin-5(2H)-ones

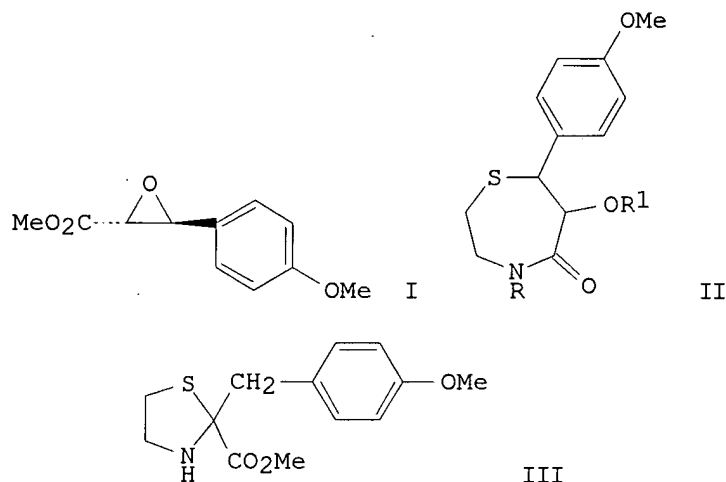
AUTHOR(S): Mohacsi, Erno; O'Brien, Jay P.; Todaro, Louis J.  
CORPORATE SOURCE: Roche Res. Cent., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA

SOURCE: Journal of Heterocyclic Chemistry (1992), 29(1), 193-7  
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Reaction of 2-aminoethanethiol with trans-3-(p-methoxyphenyl)glycidate (I) gave the (+-)-cis-1,4-thiazepinone II (R = R1 = H) and a byproduct III. The structure of II (R = R1 = H) was proven by x-ray crystallog. The x-ray data revealed that this compd. adopts the chair conformation in the solid state and the heterocyclic ring is seven-membered. The structure of the byproduct III was elucidated on the basis of spectral data. II (R = CH2CH2NMe2, R1 = H, Ac) were inactive as calcium channel blocking agents.

IT 142011-35-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

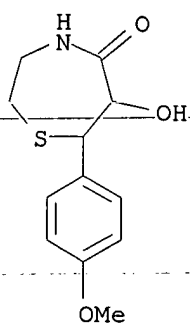
(prepn., alkylation with (dimethylamino)ethyl chloride and crystal and mol. structure of)

RN 142011-35-6 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-6-hydroxy-7-(4-methoxyphenyl)- (9CI)  
(CA INDEX NAME)



09/836,548



~~113~~ ANSWER 12 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:106251 CAPLUS

DOCUMENT NUMBER: 116:106251

TITLE: The base-promoted dehydration of racemic trans-tetrahydro-6-hydroxy-4-[(2-(dimethylamino)ethyl)-7-(4-methoxyphenyl)-1,4-thiazepin-5(2H)-one

AUTHOR(S): Mohacsi, Erno; O'Brien, Jay P.

CORPORATE SOURCE: Roche Res. Cent., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA

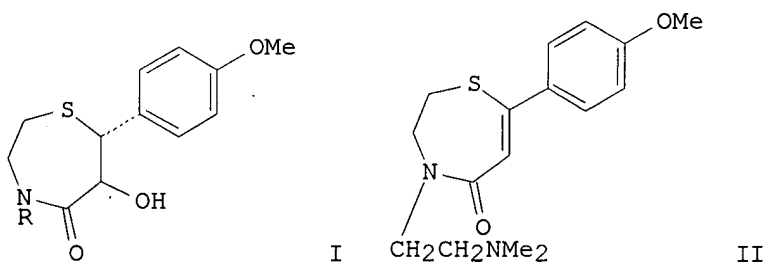
SOURCE: Journal of Heterocyclic Chemistry (1991), 28(8), 2051-2

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The base-catalyzed alkylation of racemic-trans-hydroxy(methoxyphenyl)thiazepinone I (R = H) with dimethylaminoethyl chloride in DMSO provided predominantly I (R = CH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>) and also dihydro[(dimethylamino)ethyl](methoxyphenyl)thiazepinone II.

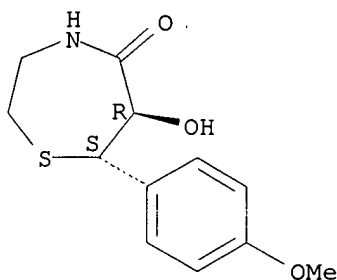
IT 130056-74-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(alkylation of, with (dimethylamino)ethyl chloride)

RN 130056-74-5 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-6-hydroxy-7-(4-methoxyphenyl)-, trans-(9CI) (CA INDEX NAME)

Relative stereochemistry.



09/836,548

113 ANSWER 13 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1991:491900 CAPLUS

DOCUMENT NUMBER: 115:91900

TITLE: Novel synthesis of thianonanam using sulfur dichloride as a sulfur transfer reagent

AUTHOR(S): Komatsu, Mitsuo; Mohri, Masaaki; Kume, Shoichiro; Ohshiro, Yoshiki

CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, 565, Japan

SOURCE: Heterocycles (1991), 32(4), 659-62

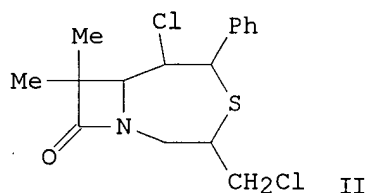
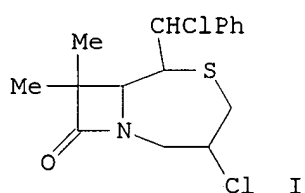
CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 115:91900

GI



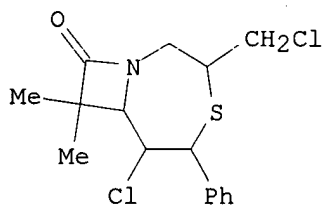
AB Thianonanams I and II were synthesized by addn. of  $\text{SCl}_2$  to N-allyl-.beta.-styryl-.beta.-lactam.

IT 135299-43-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 135299-43-3 CAPLUS

CN 4-Thia-1-azabicyclo[5.2.0]nonan-9-one, 6-chloro-3-(chloromethyl)-8,8-dimethyl-5-phenyl- (9CI) (CA INDEX NAME)



09/836,548

~~113~~ ANSWER 14 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1990:591311 CAPLUS

DOCUMENT NUMBER: 113:191311

TITLE: Synthesis and stereochemistry of rac.-trans-tetrahydro-6-hydroxy-7-(4-methoxyphenyl)-1,4-thiazepin-5(2H)-one

AUTHOR(S): Mohacsi, Erno; O'Brien, Jay P.; Todaro, Louis J.

CORPORATE SOURCE: Chem. Res. Dep., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA

SOURCE: Journal of Heterocyclic Chemistry (1990), 27(4), 1085-89

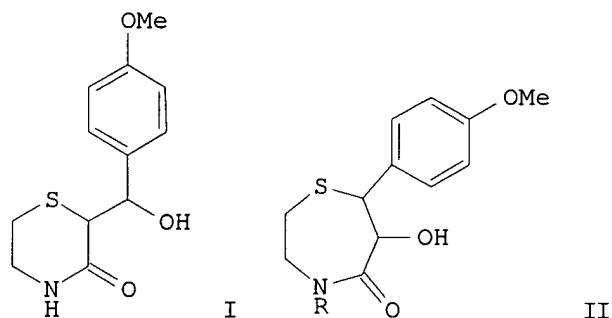
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:191311

GI



AB The base catalyzed reaction of  $\text{NH}_2\text{CH}_2\text{CH}_2\text{SH}$  with Me trans-3-(p-methoxyphenyl)glycidate gave a mixt. of isomeric lactams I and II ( $\text{R} = \text{H}$ ) and in addn., a byproduct 4H-2,3,5,6-tetrahydro[1,3]thiazin-3-one. The structures of I and II ( $\text{R} = \text{CH}_2\text{CH}_2\text{NMe}_2$ ) were detd. by x-ray crystallog. The data revealed that both isomers adopt the chair conformation in the solid state.

IT **130056-74-5P**

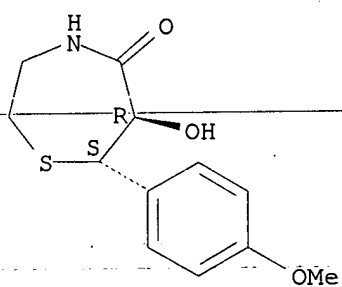
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 130056-74-5 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-6-hydroxy-7-(4-methoxyphenyl)-, trans-(9CI) (CA INDEX NAME)

Relative stereochemistry.

09/836,548



113 ANSWER 15 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1987:617608 CAPLUS

DOCUMENT NUMBER: 107:217608

TITLE: Ring-contraction reactions of dihydro- and tetrahydrothiazepines to isothiazolone derivatives

under Pummerer conditions

AUTHOR(S): Yamamoto, Kagetoshi; Yamazaki, Shoko; Murata, Ichiro; Fukazawa, Yoshimasa

CORPORATE SOURCE: Fac. Sci., Osaka Univ., Toyonaka, 560, Japan

SOURCE: Journal of Organic Chemistry (1987), 52(23), 5239-43

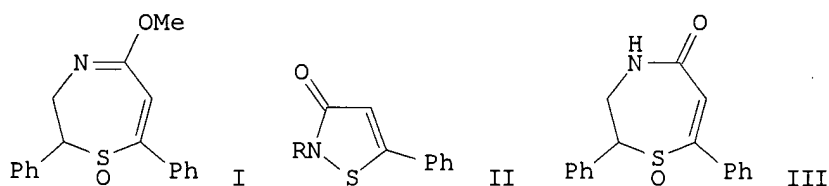
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 107:217608

GI



AB Thiazepine oxide I underwent Pummerer reaction (NaOAc in Ac<sub>2</sub>O) to give styrylisothiazole II (R = cis-PhCH:CH) which isomerized to the trans-isomer upon heating. Similarly, sulfoxide III underwent ring contraction to give II (R = trans-PhCH:CH) and 2-acetoxy-4,5-diphenylpyridine. However, upon treatment with (CF<sub>3</sub>CO)<sub>2</sub>O, III gave oxoisothiazole II [R = PhCH(O<sub>2</sub>CCF<sub>3</sub>)CH<sub>2</sub>]. A mechanism for these ring contractions, which involves a common bicyclic intermediate, is suggested.

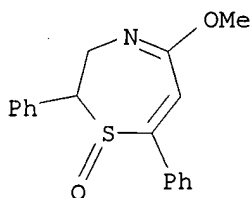
IT 110567-89-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and Pummerer reaction of, phenylstyrylisothiazole from)

RN 110567-89-0 CAPLUS

CN 1,4-Thiazepine, 2,3-dihydro-5-methoxy-2,7-diphenyl-, 1-oxide (9CI) (CA INDEX NAME)



IT 110567-92-5P

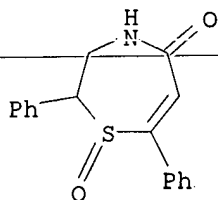
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and Pummerer reaction of, with acetic anhydride or trifluoroacetic anhydride)

RN 110567-92-5 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-2,7-diphenyl-, 1-oxide (9CI) (CA

INDEX NAME)

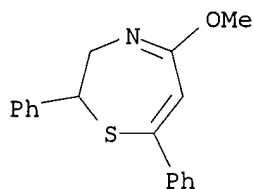


IT 110567-88-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and chloroperbenzoic acid oxidn. of)

RN 110567-88-9 CAPLUS

CN 1,4-Thiazepine, 2,3-dihydro-5-methoxy-2,7-diphenyl- (9CI) (CA INDEX NAME)

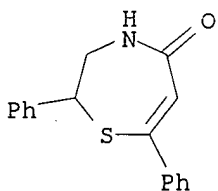


IT 110567-87-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn., chloroperbenzoic acid oxidn., or O-methylation of, with  
trimethyloxonium tetrafluoroborate)

RN 110567-87-8 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-2,7-diphenyl- (9CI) (CA INDEX NAME)



09/836,548

~~LIB~~ ANSWER 16 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1986:608947 CAPLUS

DOCUMENT NUMBER: 105:208947

TITLE: 1,4-Thiazepinethiones as plant fungicides

INVENTOR(S): Nishihata, Takeshi; Saito, Toshinori; Yasufuku, Kazue;

Fukatsu, Shunzo; Matsumoto, Kuniomi; Watanabe, Tetsuo

PATENT ASSIGNEE(S): Meiji Seika Kaisha, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

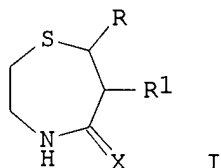
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61083176	A2	19860426	JP 1984-206015	19841001

OTHER SOURCE(S): CASREACT 105:208947  
GI



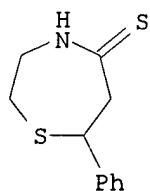
AB The title compds. [I; R, R1 = H, C1-5 alkyl, (substituted) aryl, aralkyl; X = S], useful as plant fungicides, were prepd., e.g., by treating I (X = O) with P2S5 or Lawesson's reagent. Thus, heating a suspension of 1.73 g I (R = CHMe2, R1 = H, X = O) in 70 mL pyridine with 2.31 g P2S5 at 90.degree. for 30 min gave 0.75 g I (R = CHMe2, R1 = H, X = S), which was as effective as Hinosan against rice blast.

IT 105150-99-0P 105151-01-7P 105151-02-8P  
105151-03-9P 105151-05-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as plant fungicide)

RN 105150-99-0 CAPLUS

CN 1,4-Thiazepine-5(2H)-thione, tetrahydro-7-phenyl- (9CI) (CA INDEX NAME)

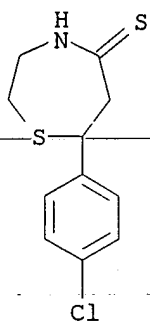


RN 105151-01-7 CAPLUS

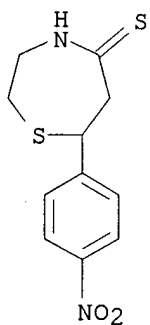
CN 1,4-Thiazepine-5(2H)-thione, 7-(4-chlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)



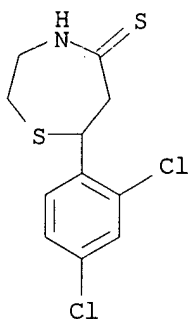
09/836,548



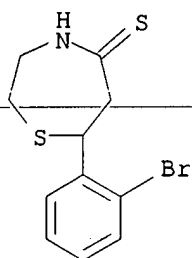
RN 105151-02-8 CAPLUS  
CN 1,4-Thiazepine-5(2H)-thione, tetrahydro-7-(4-nitrophenyl)- (9CI) (CA  
INDEX NAME)



RN 105151-03-9 CAPLUS  
CN 1,4-Thiazepine-5(2H)-thione, 7-(2,4-dichlorophenyl)tetrahydro- (9CI) (CA  
INDEX NAME)



RN 105151-05-1 CAPLUS  
CN 1,4-Thiazepine-5(2H)-thione, 7-(2-bromophenyl)tetrahydro- (9CI) (CA INDEX  
NAME)



IT 2897-03-2 105151-08-4 105151-09-5

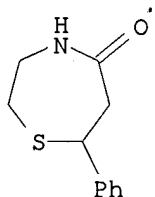
105151-10-8 105151-12-0

RL: RCT (Reactant)

(sulfuration of, with phosphorus pentasulfide)

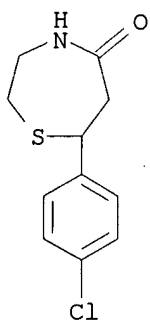
RN 2897-03-2 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 105151-08-4 CAPLUS

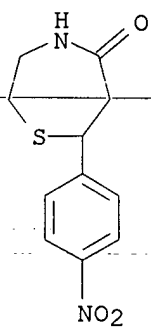
CN 1,4-Thiazepin-5(2H)-one, 7-(4-chlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)



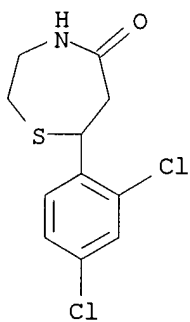
RN 105151-09-5 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

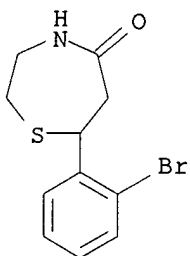
09/836,548



RN 105151-10-8 CAPLUS  
CN 1,4-Thiazepin-5(2H)-one, 7-(2,4-dichlorophenyl)tetrahydro- (9CI) (CA  
INDEX NAME)



RN 105151-12-0 CAPLUS  
CN 1,4-Thiazepin-5(2H)-one, 7-(2-bromophenyl)tetrahydro- (9CI) (CA INDEX  
NAME)



~~13~~ ANSWER 17 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1981:15694 CAPLUS

DOCUMENT NUMBER: 94:15694

TITLE: Investigation of the reaction products of  
5-amino-1,3-disubstitutedpyrazoles with aromatic  
aldehydes. Synthesis of new fluorinated  
1,3,4-trisubstituted-1H-pyrazolo[3,4-e][1,4]thiazepin-  
7-ones

AUTHOR(S): Joshi, Krishna C.; Pathak, Vijai N.; Garg, Urmila

CORPORATE SOURCE: Dep. Chem., Univ. Rajasthan, Jaipur, 302004, India

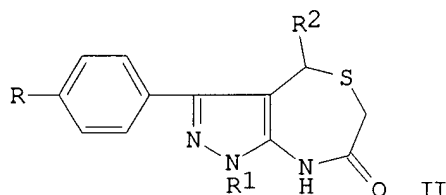
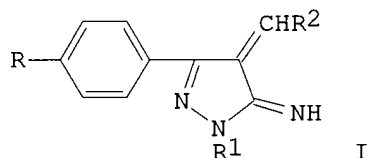
SOURCE: J. Heterocycl. Chem. (1980), 17(4), 789-91

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



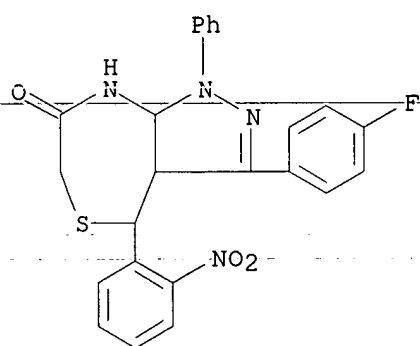
AB The condensation products of 1,3-disubstituted 5-aminopyrazoles with arom. aldehydes were identified as phenylmethylenepyrazolimine derivs. I (R = F, H, R1 = Ph, p-ClC6H4, p-FC6H4, C6F4, p-MeC6H4SO2, p-FC6H4SO2; R2 = substituted Ph). Treatment I with mercaptoacetic acid gave new fluorine contg. pyrazolothiazepinones II.

IT **76058-84-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and proton and fluorine-19 NMR of)

RN 76058-84-9 CAPLUS

CN 1H-Pyrazolo[3,4-e][1,4]thiazepin-7(6H)-one, 3-(4-fluorophenyl)-3a,4,8,8a-tetrahydro-4-(2-nitrophenyl)-1-phenyl- (9CI) (CA INDEX NAME)



13 ANSWER 18 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1980:408144 CAPLUS

DOCUMENT NUMBER: 93:8144

TITLE: Chlorination-dehydrochlorination of  
perhydro-1,4-thiazepin-5-ones

AUTHOR(S): Wamhoff, Heinrich; Theis, Christoph H.

CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300/1,  
Fed. Rep. Ger.

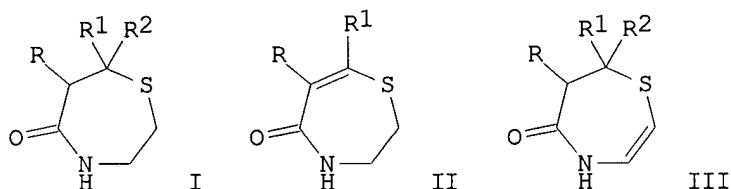
SOURCE: Chem. Ber. (1980), 113(3), 995-1009

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

GI



AB Chlorination of the thiazepinones I ( $R = R_2 = H$ ,  $R_1 = H$ , Me, Ph, 4-MeOC<sub>6</sub>H<sub>4</sub>;  $R = Me$ , Ph,  $R_1 = R_2 = H$ ;  $R = H$ ,  $R_1 = R_2 = Me$ ) with SO<sub>2</sub>Cl<sub>2</sub> or N-chlorosuccinimide, followed by dehydrochlorination, gave II and III. Reaction with Me<sub>3</sub>COCl gave the S-oxides of I in addn. to the chlorination products. Halogenation of II ( $R = H$ ,  $R_1 = H$ , Me, Ph) with SO<sub>2</sub>Cl<sub>2</sub> or Br gave II ( $R = Cl$ , Br).

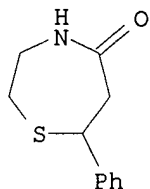
IT 2897-03-2

RL: RCT (Reactant)

(chlorination-dehydrochlorination of)

RN 2897-03-2 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

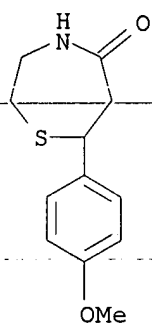


IT 73920-60-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and chlorination-dehydrochlorination of)

RN 73920-60-2 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

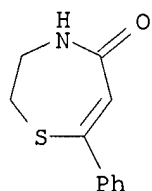


IT **65922-92-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and halogenation of)

RN 65922-92-1 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-7-phenyl- (9CI) (CA INDEX NAME)

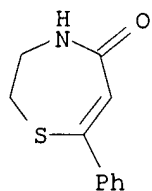


IT **73920-73-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and neutralization of)

RN 73920-73-7 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-7-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



HCl

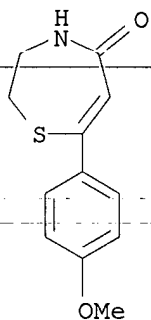
IT **73920-66-8P 73920-74-8P 73920-79-3P**

**73920-81-7P 73920-82-8P**

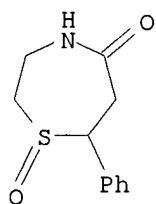
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 73920-66-8 CAPLUS

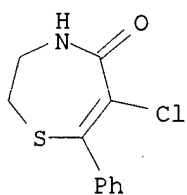
CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



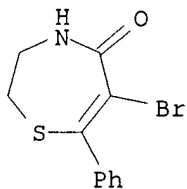
RN 73920-74-8 CAPLUS  
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-phenyl-, 1-oxide (9CI) (CA INDEX NAME)



RN 73920-79-3 CAPLUS  
CN 1,4-Thiazepin-5(2H)-one, 6-chloro-3,4-dihydro-7-phenyl- (9CI) (CA INDEX NAME)



RN 73920-81-7 CAPLUS  
CN 1,4-Thiazepin-5(2H)-one, 6-bromo-3,4-dihydro-7-phenyl- (9CI) (CA INDEX NAME)

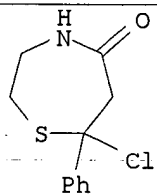


RN 73920-82-8 CAPLUS



09/836,548

CN 1,4-Thiazepin-5(2H)-one, 7-chlorotetrahydro-7-phenyl- (9CI) (CA INDEX  
NAME)



~~LA3~~ ANSWER 19 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1978:152525 CAPLUS

DOCUMENT NUMBER: 88:152525

TITLE: Antihypertensive agents: Part V. Synthesis and antihypertensive activity of 3-arylimino-2,3,5,6-tetrahydro-4H-1,4-thiazines and related cyclic amidines

AUTHOR(S): Arya, V. P.; Kaul, C. L.; Grewal, R. S.; David, J.; Talwalker, P. K.; Shenoy, S. J.

CORPORATE SOURCE: Res. Cent., Ciba-Geigy, Bombay, India

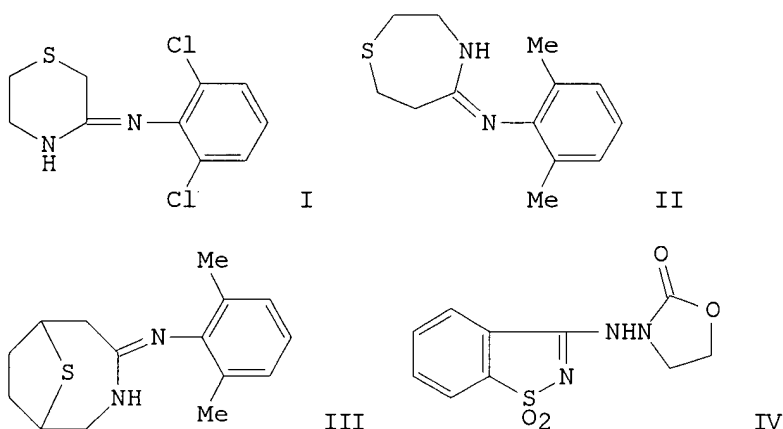
SOURCE: Indian J. Chem., Sect. B (1977), 15(8), 720-6

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



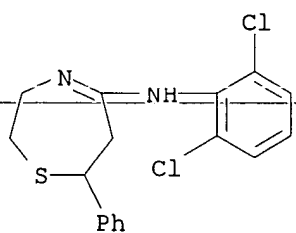
AB 3-Arylimino-2,3,5,6-tetrahydro-4H-1,4-thiazines, e.g., I, were prepd. from thiamorpholin-3-one, POCl<sub>3</sub>, and anilines for antihypertensive screening. The corresponding 1,4-oxazines were prepd. from substituted morpholin-3-ones, POCl<sub>3</sub>, and substituted anilines. Seven- and eight-membered cyclic amidines, e.g., II, were prepd. by treating the corresponding lactams with POCl<sub>3</sub> and substituted anilines. A novel heterocyclic amidine III, was prepared from tropinone; IV was also prepd. The structure-activity relationship of the cyclic amidines was reported.

IT **65922-96-5P**

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(prepn. and antihypertensive activity of)

RN 65922-96-5 CAPLUS

CN 1,4-Thiazepin-5-amine, N-(2,6-dichlorophenyl)-2,3,6,7-tetrahydro-7-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



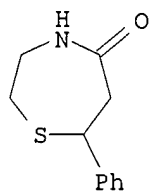
● HCl

IT **2897-03-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and condensation with anilines)

RN 2897-03-2 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

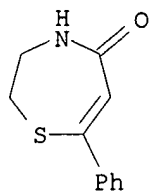


IT **65922-92-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and condensation with dimethylaniline)

RN 65922-92-1 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-7-phenyl- (9CI) (CA INDEX NAME)



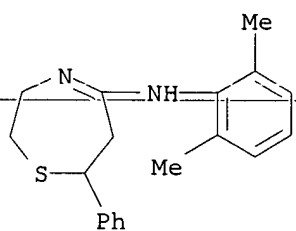
IT **65922-97-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and pharmacol. activity of)

RN 65922-97-6 CAPLUS

CN 1,4-Thiazepin-5-amine, N-(2,6-dimethylphenyl)-2,3,6,7-tetrahydro-7-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

09/836,548



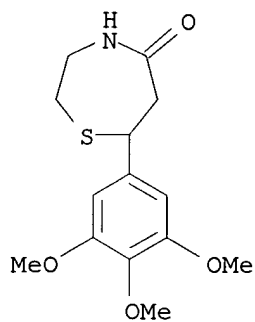
● HCl

IT 65922-91-0P 65923-18-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

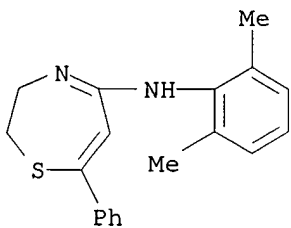
RN 65922-91-0 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



RN 65923-18-4 CAPLUS

CN 1,4-Thiazepin-5-amine, N-(2,6-dimethylphenyl)-2,3-dihydro-7-phenyl-,  
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

✓ 13 ANSWER 20 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1976:165182 CAPLUS  
 DOCUMENT NUMBER: 84:165182  
 TITLE: Synthesis of some dehydrophenylalanine peptides  
 AUTHOR(S): Breitholle, Edward G.; Stammer, Charles H.  
 CORPORATE SOURCE: Chem. Dep., Univ. Georgia, Athens, Ga., USA  
 SOURCE: J. Org. Chem. (1976), 41(8), 1344-9  
 CODEN: JOCEAH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

GI For diagram(s), see printed CA Issue.

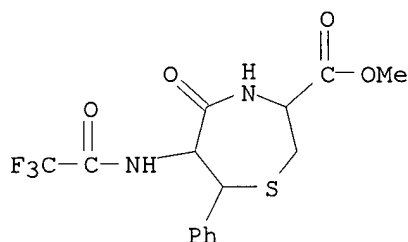
AB Addnl. data considered in abstracting and indexing are available from a source cited in the original document. The bromo pseudoazlactones, (I, R1 = H, Me, Ph, Me2CH, Et, R2 = H, Me), dehydrobrominated readily giving the unsatd. azlactones, II, which were converted into N-trifluoroacetyldehydro amino acid anilides and peptides and perhydro-1,4-thiazepin-5-ones. N-trifluoroacetyldehydrovaline, isoleucine, leucine, alanine, and aminobutyric acid anilides and peptides were not deblocked by NH3. Treatment of I (R1 = Ph, R2 = H) in DMF contg. Et3N with Phe-OMe gave 76% PhCH:C(NHCOCF3)CONHCH(CH2Ph)CO2Me.

IT **58219-84-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 58219-84-4 CAPLUS

CN 1,4-Thiazepine-3-carboxylic acid, hexahydro-5-oxo-7-phenyl-6-  
 [(trifluoroacetyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



113 ANSWER 21 OF 21 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1975:3907 CAPLUS

DOCUMENT NUMBER: 82:3907

TITLE: Reaction products from 4-phenylbut-3-yn-2-one and aliphatic diamines or 2-aminoethanethiol, and from 2-aminoethanethiol and .alpha.,.beta.-enones

AUTHOR(S): Hankovszky, Olga H.; Hideg, Kalman; Lloyd, Douglas

CORPORATE SOURCE: Cent. Lab. Chem., Univ. Pecs, Pecs, Hung.

SOURCE: J. Chem. Soc., Perkin Trans. 1 (1974), (14), 1619-21  
CODEN: JCPRB4

DOCUMENT TYPE: Journal

LANGUAGE: English

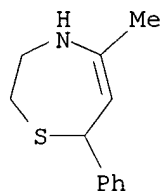
AB PhC.tplbond.CCOME with H<sub>2</sub>N(CH<sub>2</sub>)<sub>n</sub>NH<sub>2</sub> (n = 2, 3) in the presence and absence of Na<sub>2</sub>CO<sub>3</sub> gave MeCOCH:CPhNH(CH<sub>2</sub>)<sub>n</sub>NHCPh:CHCOMe and PhC.tplbond.CCMe:N(CH<sub>2</sub>)<sub>n</sub>N:CMcC.tplbond.CPh, resp. H<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>SH with PhC.tplbond.CCOME gave MeCOCH:CPhNH(CH<sub>2</sub>)<sub>2</sub>SH, with PhCH:CHCOMe gave 2,3,6,7- and/or 2,3,4,7-tetrahydro-5-methyl-7-phenyl-1,4-thiazepine, and with chalcone gave PhCOCH<sub>2</sub>CHPhNH(CH<sub>2</sub>)<sub>2</sub>SH and PhCOCH<sub>2</sub>CHPhS(CH<sub>2</sub>)<sub>2</sub>NH<sub>2</sub> or PhCOCH<sub>2</sub>CHPhS(CH<sub>2</sub>)<sub>2</sub>NHCHPhCH<sub>2</sub>COPh depending on the molar ratios used.

IT 54454-44-3P 54454-45-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 54454-44-3 CAPLUS

CN 1,4-Thiazepine, 2,3,4,7-tetrahydro-5-methyl-7-phenyl- (9CI) (CA INDEX NAME)



RN 54454-45-4 CAPLUS

CN 1,4-Thiazepine, 2,3,6,7-tetrahydro-5-methyl-7-phenyl- (9CI) (CA INDEX NAME)

